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INTELLIGENT/ADAPTIVE SITE CHARACTERIZATION SOFTWARE

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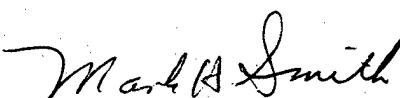
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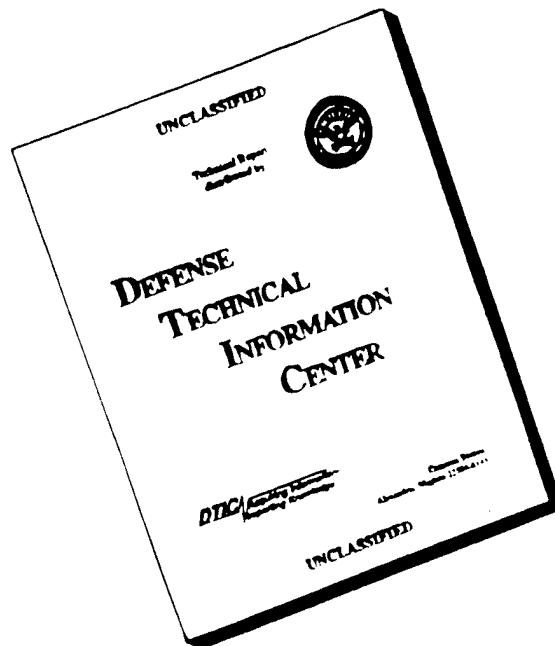
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13. ABSTRACT *(Maximum 200 words)*

A computer based analysis package was developed to assist field personnel conducting environmental site characterization projects. Applied Research Associates, Inc. conducted the research project for the Air Force and were assisted by researchers at the University of Vermont, Colorado School of Mines, Argonne National Laboratory and ConSolve Inc. of Lexington MA.. The goal of the project was to develop a user friendly software system which could be used to analyze field data in near real time and to select additional sampling points based on the prior data set. The software package, entitled IASite (Intelligent/Adaptive-Site Characterization) is designed to run on a high end IBM compatible PC with a minimum of 32 Megabytes of memory and one gigabyte of hard disc space. As of the date of the project, many of the available geostatistical codes and environmental site characterization database programs only run on the UNIX operating system, hence the PC computer is set up to operate with both a UNIX and Windows operating system. The I/A-Site software package is designed to be modular so that different analysis or graphics programs can be added as desired. Major software components of I/A-Site include: SitePlanner® from ConSolve which serves as the data base, links the various software packages and provides 2-D graphics capability, ConeTap, from ARA which analyzes CPT data and provides the data in a format compatible for use by I/A-Site, three geostatistical codes (PLUME developed by Argonne National Laboratory, SCANN developed by the University of Vermont, and UNCERT developed by the Colorado School of Mines). A probabilistic groundwater flow code (POWDER, developed by UVM) is also provided as is the 3-D graphics program SiteView developed by ConSolve. The final software tool provided is OSCAR, developed by ARA, which is a cost optimization program to determine when sufficient site characterization data has been collected. The software packages can be addressed in a X-Windows environment and data from a variety of formats (i.e. Excel spreadsheets, etc.) can be imported or exported.

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PREFACE

This report was prepared by Applied Research Associates, Inc., 120-A Waterman Road, South Royalton, Vermont 05068, under Contract No. FO86-93-C-0020 for the Armstrong Laboratory Environics Directorate (AL/EQ), Suite 2, 139 Barnes Drive, Tyndall Air Force Base, Florida 32403-5319.

This report describes the Intelligent/Adaptive Site Characterization System. The work was performed between September 1993 and July 1995. The AL/EQW project officer was Bruce Nielsen.

EXECUTIVE SUMMARY

A. OBJECTIVE

The goal of this effort was to develop an intelligent/adaptive site characterization system that would reduce cost and increase efficiencies of the site characterization process. This system incorporates real-time data analysis methods into the site characterization process. An adaptive site characterization methodology is defined as a method that can optimize the use of surface geophysical and cone penetrometer probe measurements, as well as traditional drilling, sampling and monitoring techniques. An intelligent methodology involves interaction between predictive mathematical models and site measurements to both improve the predictions and make optimal decisions regarding the site measurements. The developed system integrates both of these key concepts to make the site characterization process as efficient and cost-effective as possible.

B. BACKGROUND

The Departments of Defense and Energy are conducting nationwide remediation efforts to clean up contaminated military, national laboratory and weapons facilities. Contamination ranges from gasoline, diesel fuel, solvents and domestic waste to highly hazardous contaminants such as radioactive waste, explosives and toxic gases. It has been estimated that remediation of DOE sites will require expenditure of $200-$250 billion dollars over 30 years. The best estimate of DOD costs to clean up military facilities is $24 billion dollars, with Super-Fund sites costing $230 billion and RCRA corrective actions expected to cost $230 billion (1). The Air Force alone has identified over 4,300 hazardous waste sites and 300 inactive firefighting training facilities as part of the Installation Restoration Program Information Management System (IRPIMS); the IRPIMS database contains data from only one-half of the Air Force installations (2). Identifying, characterizing and developing remediation plans for these contaminated sites is a high priority of both the DOD and DOE.

Environmental site characterization approaches, even to this date, are usually based on traditional drilling, sampling and laboratory testing. Characterization plans are formulated on informed judgment that considers site geology, the characterization requirements, and, perhaps, information available from previous wells, or drilling logs from previous investigations. The traditional approach involves laying out an array of drill holes, often in a rectangular pattern, with spacing determined from judgment or rules of thumb. Cuttings are examined in the field and samples are taken to the laboratory for testing and analysis. After a few weeks to several months, the scientists/engineers are able to assess the results of their plan. They can then order in-fill drill holes and monitoring wells. Plume characterization, because of its three-dimensional nature, usually requires significant in-fill sampling and well monitoring, adding additional time and cost to the investigation. The traditional environmental site investigation process is nearly stalled by the slowness of drilling, the lengthy times for laboratory testing and, overall lack of real-time decision-making capability. The DOD and DOE have recognized that, to meet their cleanup time tables, the traditional Remediation Investigation and Feasibility Study (RI/FS) approach is inadequate.

C.   SCOPE

With the wide range of problems to be encountered by the DOD and DOE, it is highly unlikely that one set of predictive tools will be adequate for all site conditions. The geologic setting, type of contaminant, and remediation approach all dictate that a range of predictive tools will be required. Therefore our approach is to develop a basic set of software tools which can be used to:

- Evaluate the contaminant distribution and site stratigraphy,
- Locate subsequent sounding and sampling locations,
- Provide a data base of all pertinent site data,
- Graphically display all site data, and

- ·Assist in evaluating if sufficient data exists to adequately define the contaminated zone.

The software was developed is such a way that other predictive codes (i.e., hydrogeologic or contaminant transport) can be readily incorporated, thereby allowing users of the software package to include those predictive software packages that best solve **their** particular problem.

D.   RESULTS AND CONCLUSIONS

The result of this research program is a software package titled I/A-Site. The I/A-Site software package is designed to be modular so that additional analysis or graphics programs can be added as desired. Major software components of I/A-Site include: (1) SitePlanner® from ConSolve, which serves as the data base, links the various software packages and provides 2-D graphics capability; (2) ConeTap from ARA, which analyzes CPT data and provides the data in a format compatible for use by I/A-Site, and (3) three geostatistical codes (PLUME developed by Argonne National Laboratory, SCANN developed by the University of Vermont, and UNCERT, developed by the Colorado School of Mines). A probabilistic groundwater flow code, POWDER, developed by UVM is also provided, as is the 3-D graphics program SiteView developed by ConSolve. The final software code provided is OSCAR, developed by ARA which is a cost-optimization program to determine when sufficient site characterization data have been collected. The software packages can be addressed in an X-Windows environment and data from a variety of formats (i.e. Excel spreadsheets, etc.) can be imported or exported.

The IASite software system can take all current knowledge concerning a site and graphically display this data. The system extends further than data visualization with the incorporation of a variety of tools to assist the engineer in selecting optimal test locations and making informed decisions concerning further testing activities. Furthermore the software will assist the engineer in determining if the costs of additional testing are justified while considering total cleanup costs and the accuracy levels required. The use of these types of tools facilitates

more effective site characterization. Capabilities which have been incorporated into the IASite software include:

- The ability to store and recall a diverse data set, including analytical results, drilling logs, geologic descriptions, results from geophysical testing etc.

- A simple to easy-to-use graphic system to develop overlay plots of the diverse data set to show trends in the data and correlations.

- The ability to analyze and display the massive amounts of CPT data to determine important soil information.

- Geostatistical methods to develop maps of interest parameters, such as soil stratigraphy, water table surface, plume boundaries and concentrations, and the uncertainties of these properties.

- Decision analysis tools to assist field personnel in selecting new test locations, deciding the types of data to be obtained and evaluating additional data.

- A groundwater flow and transport model to assist in estimates of likely contaminate flow patterns, plume location and shape.

- Three-dimensional graphics system for use in the analysis of plume shape and presentation of results.

H.   RECOMMENDATIONS

At the time when IASite was developed, significant software limitations existed on the PC platform and the Windows operating system. Since the project completion, Windows 95 has been released which solves many of these limitations. In addition, inexpensive Graphical Information System developed for the PC can replace the UNIX-based SitePlanner® graphical-data-based program.

Due to these changes it is recommended that the IASite program be converted to Windows 95 and incorporate a Windows-based GIS database program and to fully integrate all of

the software programs as 32-bit application. This will increase the speed of the analysis programs and bring all of the applications over to one operating system platform on the PC.

An additional recommendation is that the software be tested under field conditions and modified as required. This phase of the software development program was eliminated from the original program and IASite has not been fully evaluated in the field. The cost simulation model incorporated in the system represents an initial simple model, and additional models should be evaluated. These models could incorporate more complex penalty costs and also consider concepts of risk-based use issues.

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SECTION I

INTRODUCTION

A. OBJECTIVE

This document represents the final report for an intelligent/adaptive site characterization software system developed by Applied Research Associates, Inc. under contract to Armstrong Laboratories of the US Air Force. The goal of the software system is to assist engineering personnel in the real-time analysis and decision making aspects of site characterization activities. The system can store and graphically display all available information concerning a site. The system expands upon data visualization with the incorporation of a variety of tools to assist the engineer in selecting optimal test locations and making informed decisions concerning further testing activities. Furthermore the software assists the engineer in determining if the costs of additional testing are justified while considering total cleanup costs and the accuracy levels required. The use of these tools increases the effectiveness and efficiency of the intelligent/adaptive site characterization process.

B. PROBLEM BACKGROUND

The Departments of Defense and Energy are conducting nationwide remediation efforts to clean up contaminated military, national laboratory and weapons facilities. The range of sites requiring remediation is far more diverse than that found in the commercial sector, and includes sites located in urban settings and extremely remote locations. Contamination ranges from gasoline, diesel fuel, solvents and domestic waste to highly hazardous contaminants such as radioactive waste, explosives, and toxic gases. It has been estimated that remediation of DOE sites will require expenditure of $200-$250 billion dollars over 30 years. The best estimate of DOD costs to clean up military facilities is $24 billion dollars, with Super-Fund sites costing $230 billion and RCRA corrective actions expected to cost $230 billion (1). The Air Force alone

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has identified over 4,300 hazardous waste sites and 300 inactive firefighting training facilities as part of the Installation Restoration Program Information Management System (IRPIMS); the IRPIMS database contains data from only one-half of the Air Force installations (2). Identifying, characterizing and developing remediation plans for these contaminated sites is a high priority of both the DOD and DOE.

Environmental site characterization approaches, even to this date, are usually based on traditional drilling, sampling and laboratory testing. Characterization plans are formulated on informed judgment that considers site geology, the characterization requirements, and, perhaps, prior information available from previous wells, or drilling logs from previous investigations. The traditional approach involves laying out an array of drill holes, often in a rectangular pattern, with spacing determined from judgment or rules of thumb. Cuttings are examined in the field and samples are taken to the laboratory for testing and analysis. After a few weeks to several months, the scientists/engineers are able to assess the results of their plan. They can then order in-fill drill holes and monitoring wells. Plume characterization, because of its three dimensional nature, usually requires significant in-fill sampling and well monitoring, adding additional time and cost to the investigation. The traditional environmental site investigation process is nearly stalled by the slowness of drilling, the lengthy times for laboratory testing and, overall lack of real-time decision-making capability. The DOD and DOE have recognized that to meet their cleanup time tables, the traditional Remediation Investigation and Feasibility Study (RI/FS) approach is inadequate.

To address the problems with the traditional RI/FS process, the DOD and DOE are pursuing broad-based research, development and demonstration programs in the area of environmental site characterization and remediation. Tools are being developed to characterize a site more rapidly, using less invasive techniques such as Cone Penetration Technology (CPT) and real-time sensors deployed on the CPT. In addition, less invasive in situ site remediation techniques are being developed such as soil venting, bioremediation, radio frequency heating and electrokinetic methods. Advantages of this approach are that the necessary time required to

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complete the site evaluation and design the remediation process is reduced, less waste is generated, and the political problems associated with transporting the waste off-site for either incineration or burial are eliminated. In addition, this approach results in less potential damage to the environment.

Research programs by the DOD and DOE in this area are in direct response to the need for the identification and characterization of contaminated sites in a more timely and economical manner than currently possible with traditional drilling, sampling and laboratory testing techniques (3 and 4). The ultimate goal of these research programs is to develop a more complete contaminant distribution and geologic model which can be used to design more cost-effective remediation plans. As a result of this work, significant limitations in currently available site characterization equipment and analysis methods have been identified, and programs have been created to develop the much needed improvements. The Tri-Service agreement to develop the Site Characterization and Analysis Penetration System (SCAPS) and the Air Force developed tunable dye laser system are examples of the DOD and DOE efforts to develop advanced field characterization tools (2).

Efforts to date have been devoted to developing tools for rapid in situ measurement of parameters that have typically been measured in the laboratory and in developing in situ treatment methods. Site characterization tools being developed include field portable gas chromatographs, mass spectrometers, multigas monitors, radiation detectors, organic vapor monitors and fiber-optic probes for detecting both fuel and chlorinated hydrocarbon contaminants. The first implementation of these measurement systems was with conventional drilling. With their faster response time, (most offer real time measurements of the contaminant concentrations) many of these systems are being adapted to the more rapid, less invasive CPT. By coupling the CPT with advanced sensor technology, it is now possible to obtain estimates of the contaminant distribution every 2 cm, whereas drilling measurements are typically obtained at 5-foot depth intervals. These programs have been very successful, and it is now possible to

achieve field screening measurements in near real-time, whereas previously, these results may have required weeks.

These research programs have greatly reduced the time required to acquire data and have greatly improved the data density. However, the methods to analyze these data are essentially the same as were used 10 to 15 years ago. In the worst case, the engineer/scientist manually sifts through reams of data and develops contours of the contaminant plume using contouring programs. In the best case, the engineer/scientist has access to a database and couples the database to a contouring program to "automate" the process. Drilling, sampling and analytical testing plans are still typically laid out on a rectangular grid with samples taken at set depth intervals (typically every 5 feet), or changes in lithology. These rigid plans, although typical of the industry, often miss significant areas of contamination and are wasteful of the limited financial resources. It is common to discover that a high percentage of site monitoring wells are in the area of "nondetect", are screened at the wrong depth interval, or are too shallow. Although the well may be in a nondetect region, it still must be monitored on a quarterly basis at a high cost, yet it adds no useful additional data (5).

A need exists to eliminate unproductive sampling programs. One of the leading causes of this loss of productivity is the lack of adequate field data analysis tools. Decisions regarding the initial round of sampling are usually based on limited prior knowledge and the best guess of the field personnel. The quality of this decision is a direct function of the experience level of the field personnel. With the current site characterization process delays are common, and at many sites the exploration crew is demobilized while decisions are being made regarding the next round of sampling locations. Advances in storage, analysis and presentation of the diverse set of data from a site characterization program are imperative. Desirable capabilities include:

- The ability to store and recall a diverse data set, including analytical results, drilling logs, geologic descriptions, results from geophysical testing etc.
- A simple to use graphic system to develop overlay plots of the diverse data set to show trends in the data and correlations.

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- The ability to analyze the massive amounts of CPT data to determine soil strata, contaminant concentrations and required determine material properties (i.e., hydraulic conductivity).

- Geostatistical methods to develop maps of parameters of interest, such as soil stratigraphy, water table surface, plume boundaries and concentrations, and the uncertainties of these properties.

- Decision analysis tools to assist field personnel in the selection of new data locations, the types of data to be obtained and the value of the additional data.

- Groundwater flow models to assist in estimates of likely contaminant flow patterns, plume location and shape.

- Three-dimensional graphics system for use in the analysis of plume shape and presentation of results.

The approach developed under this program attempts to combine recent sensor improvements into an improved analysis and visualization system. The intelligent/adaptive approach brings the site characterization analysis technology forward to match the recent advances in site characterization equipment. New analysis methods are developed and incorporated into the system to fulfill many of the capabilities listed above.

C.   SCOPE

This document describes the system, and is organized into four sections. The first section covers background materials such as the need for improved site characterization analysis tools. Section II presents an overview of the developed system and a list of the advantages and disadvantages concerning its use for site characterization activities. Section III presents an evaluation of the various tools used in the system as compared to the traditional approach, including cost comparisons. Section IV presents the conclusions gained through development of this system along with recommendations for future improvements. Appendix A contains the User's Guide for the system. The User's Guide includes general interfacing requirements as well

as detailed descriptions of the various tools integrated into the system. This section is designed for hands-on use of the system, and the described processes require some practice by the user.

SECTION II

OVERVIEW OF INTELLIGENT/ADAPTIVE
SITE CHARACTERIZATION SYSTEM

A.   INTRODUCTION

Current EPA procedures for RI/FS (5) make passing mention of adaptive site
characterization strategies, but there is no established quantitative approach. Although
EPA-approved field operation procedures permit geophysical approaches, they insist upon
traditional drilling, sampling and monitoring wells as the main characterization tools. With the
recent research by DOD and DOE, several of the tools required to implement the adaptive
methodology are now available.

The basis for an intelligent/adaptive site characterization scheme is the interaction
between a site model which predicts the potential extent, constituents and concentrations of
contaminants and a measurement and sampling scheme that makes measurements to evaluate the
model. To be effective an adaptive site characterization methodology must fully integrate: (1)
sampling strategy guided by geostatistical models; (2) treatment of spatial randomness,
measurement errors, and statistical uncertainties; (3) real-time decision analysis; (4) cost
considerations that reflect the cost of sampling, value of sample information, and performance
measures; and.

The goal of this effort was to develop such an intelligent/adaptive site characterization
system to reduce cost and increase efficiencies of the site characterization process. This system
incorporates real-time data analysis methods into the site characterization process. An adaptive
site characterization methodology is defined as a method that can optimize the use of surface
geophysical and cone penetrometer probe measurements, as well as traditional drilling, sampling,
and monitoring techniques. An intelligent methodology is one that involves interaction between
predictive mathematical models and site measurements to both improve the predictions and make
optimal decisions regarding the site measurements. The developed system integrates both of

these key concepts to make the site characterization process as efficient and cost-effective as possible.

With the wide range of problems to be encountered by the DOD and DOE, it is highly unlikely that one set of predictive tools will be adequate for all site conditions. The geologic setting, type of contaminant and remediation approach all dictate that a range of predictive tools will be required. Therefore our approach is to develop a basic set of software tools which can be used to:

     (1) Evaluate the contaminant distribution and site stratigraphy,

     (2) Locate subsequent sounding and sampling locations,

     (3) Provide a data base of all pertinent site data,

     (4) Graphically display all site data, and

     (5) Assist in evaluating if sufficient data exists to adequately define the

         contaminated zone.

The software was developed such that other predictive codes (i.e., hydrogeologic or contaminant transport) can be readily incorporated, thereby allowing the user of the software package to include those predictive software packages that best solve their particular problem.

A schematic of the Intelligent/Adaptive Site Characterization and Remediation process is shown in Figure 1. This flowchart begins with data collected by a variety of means, consisting of but not limited to: site reconnaissance, cone penetration testing with associated sensors, drilling to obtain samples for analytical testing, and surface geophysical methods. These data are entered into the database manager which creates a virtual site model. The database manager uses the virtual model to create site maps and fence diagrams. Geostatistical modeling will be conducted to perform parameter estimates (contour plots) and error estimates using data contained in the virtual site model. Information produced by the geostatistical model can be used in either of two independent modes, both of which involve Bayesian decision analysis. In the first mode, the
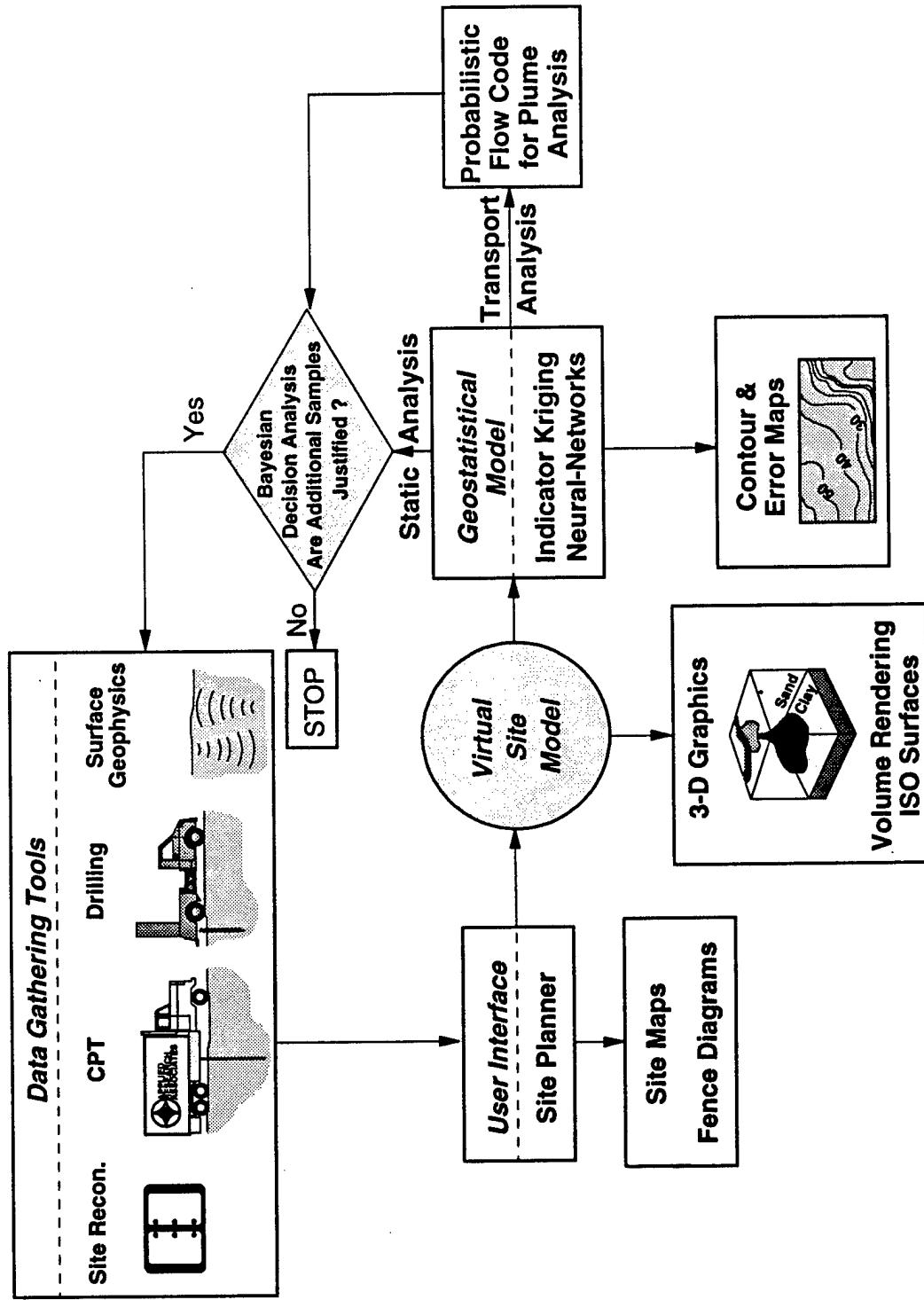
Figure 1. Flow Chart of Intelligent/Adaptive Site Characterization Process.

error maps are used to evaluate the benefits of additional measurements against the goal of the characterization plan and the cost of performing these measurements. If the costs outweigh the additional benefits of new data then the measurement process stops. The other mode can also arrive at this decision by using a flow code to estimate if the modeling errors are sufficiently small that all parameters (i.e., plume shape, contaminant concentration) are known to the appropriate confidence level. For either mode, if additional uncertainties exist then addition measurements are desired.

B.   COMPONENTS OF THE I/A-SITE SYSTEM

The major components of the software package described in the flow chart are (1) a database package, (2) a graphics package, (3) a geostatistical package, (4) a flow code, and (5) a decision analysis package. The database manager selected for this project was SitePlanner®, developed by ConSolve, Inc. of Lexington, MA, and is currently being used by DOE's Argonne National Laboratory (ANL) as the central piece of their site analysis package (6). This package creates a site model using the available data from an object-oriented database. Items from the database can easily be viewed in either table or graphically on maps, cross-sections and fence diagrams; thus SitePlanner® also assists in providing part of the graphics package. Because SitePlanner® is very easy to learn and use based upon a graphic user interface, we selected it as a core data manager software for the system.

Two different geostatistical packages are integrated into the system. The first system (UNCERT) consist of a package of tools developed at the Colorado School of Mines. Available in UNCERT are various tools for determining a variogram from the current data set, kriging tools to estimate plumes and errors associated with those plume, graphic tools for displaying results, and also simulation tools to produce numerous kriged solutions to a given input problem. UNCERT is highly versatile because various parts can be easily mixed and matched depending on the problem requirements.

The second geostatistical package is less flexible but easier to use. This code is called PLUME and was developed by Robert Johnson at Argonne National Laboratory. PLUME uses Bayesian kriging methods to determine probability maps of whether a given region is contaminated or not. Based upon these maps, the code recommends a sampling location. Once the sampling has occurred the new data are entered and the maps are updated. PLUME is able to estimate the confidence level relating to the estimated area of contamination, and testing can occur until a given confidence level is reached. PLUME also interfaces with SitePlanner® for visualization of the boring locations and probability distribution graphs.

A similar code to the two geostatistical packages is also included. This code uses an artificial neural network approach to estimate the values of various parameters over a given field. The code is named SCANN, Site Characterization using Artificial Neural Networks, and was developed by the University of Vermont. As with all artificial neural network (ANN) codes, a training set of known data is used to determine a function describing how the parameter of interest varies over the given field. The unique aspect of ANNs is that several parameters can be incorporated and weighted to determine the output variable. Operation is very simple and requires only input of the training data set to determine the plume distribution over the entire domain. The output from SCANN gives the category values of the parameter of interest over the entire range. Typically, the category values are used to represent parameter ranges such as high, medium or low or classification types such as sand, silt or clay. Tools within UNCERT can be used to display the results from SCANN.

To further advance the system a probabilistic flow code has been incorporated. This code uses a variogram developed from available site data for kriging a collection of flow fields consisting of heads and velocities. The collection of velocity fields is then used in a transport code to determine a set of potential plumes. Those plumes that do not match the original data set are then thrown out and statistics generated on those that do. Based upon the mean plume and the known variances of the plume an optimal location for the next test is selected. Although this

process is time-consuming, it is technically sound because nearly all the physics of the problem are captured in the solution method.

The final step in the process is the evaluation of the uncertainty level of the mean plume and the utility of the next sampling point. This process is performed in a code called OSCAR developed by ARA. OSCAR uses geostatistical methods to simulate a collection of plumes and a mean value plume which indicates the amount of soil that must be remediated. The selected sampling point is entered and another set of plumes generated using the probabilistic responses from that sampling event. Based upon the results of these simulations, a new quantity of soil to be remediated is generated. The total costs after testing this new location, (including sampling and cleanup), are then compared to the total costs before moving to the new location. If the costs are reduced then the new location should be tested. If two sequential locations indicate no significant decrease in total cost, the characterization phase of the project should be concluded and the remediation phase should begin. This approach is generic and allows the user to perform the analysis on a variety of parameters using any desired sampling cost or remediation cost.

In summary the intelligent/ adaptive site characterization system is highly flexible, allowing the user to solve a variety of different problems. The user can take advantage of a variety of tools to achieve the same objective, although each approach may give different results. It is the responsibility of the user to select the most appropriate method and use wise judgment in the interpretation of the results. The goal of the system is not to replace engineering judgment, but to assist the user in making more informed decisions concerning the site characterization program.

C.   STRENGTHS AND WEAKNESS OF THE APPROACH

Some major strengths of the system are listed below. Key among these is that this system represents the first time (to the author's knowledge) that a varied collection of tools have been gathered together and incorporated into a single package. This allows the user to have a

large collection of tools immediately available, rather than having to assemble the required tools for each project. In addition supplemental tools required for individual problems can easily be integrated into the system for future use. This flexibility provides the foundation for a future package that can solve problems not currently envisioned.

- Integrates a collection of tools into a single package which can be used to solve similar problems, allowing the user a variety of choices.
- Provides a user interface that simplifies input and assists the user in gathering the required data.
- Contains an integrated database for storage of all data.
- Assists the user in the determination of the level of uncertainty associated with the current status of the site characterization program, as well as a method of determining if addition sampling will reduce the total characterization and remediation costs.
- Assists the user in the selection of optimal sampling locations to reduce wasteful sampling of numerous nondetects, which ensures cost effectiveness.

Although the package has many useful features, a few limitations must be considered. The most significant is that the system can not be used blindly; proper judgment must be used to ensure that reasonable results are obtained. Poor data input generally leads to poor quality output. Other limitations include the overall size of the site to be investigated. Very large sites with large data sets, (such as entire bases), may slow the system down and reduce system performance. In these instances, each contaminated site within the base should be set up as a unique site. Care should be used to operate the software within the boundaries for which it was developed.

SECTION III

SYSTEM EVLAUATION

A.   INTRODUCTION

As described previously, a variety of tools can be used to interpolate an existing data set, create estimates of the extent of contamination, and assist with the selection of the next sampling location. Although all of these tools are available to the user, a study was performed to determine how several tools responded to a single given problem. This study provides insight into the selection of an appropriate tool for a given problem, along with guidelines for tool usage. This section documents the results of using the various mapping tools and selecting the next location. The results are compared to the traditional "by hand" methods presently used to evaluate the technical and cost benefits that can be realized using I/A-Site.

This section is divided into five subsections. The first describes the hypothetical sample problem used to evaluate the various tools. Unique aspects of the problem include an unknown source and spill date. In the second subsection, traditional engineering approaches are used to guide the investigation for the delineation of the plume. It is assumed that real-time methods are used to determine contamination presence. This allows the engineer to immediately know the results of a boring rather than waiting for laboratory analysis (which typically takes several days). This approach is more advanced than what is commonly used today, but represents the current state of the art prior to the development of the I/A-Site software system. The third subsection discusses the background and operation of the PLUME code to solve the sample problem. PLUME represents the most user-friendly of the three codes and is most likely to be used by an initial user. The SCANN code, the second easiest code to use, is discussed in the next subsection. One major weakness of SCANN is that the system must be trained on an existing data set. Therefore it would not be useful for the selection of the initial sampling locations but could be started after the completion of those locations. The cost evaluation program developed

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by ARA (OSCAR) is also presented. In this subsection we illustrate how, by using the results from the standard engineering method, the cost evaluation system can guide an investigation and assist in determining the optimal end point.

B.   SAMPLE PROBLEM

To evaluate the various tools provided in I/A-Site, a sample test case was created. The test case, depicted in Figure 2, consisted of a hypothetical unlined and uncapped landfill of 200 by 100 feet in which barrels of LNAPLs were placed. The disposal date was approximately 15 years prior to the characterization effort and site boundaries are 4,000 feet by 2400 feet.

The site flow conditions were governed by the surrounding soil materials, in this case uniform sand with a hydraulic conductivity of 5×10^{-3} cm/sec. The western site boundary was governed by a constant head boundary of 100 feet mean sea level (MSL). The eastern site boundary was also constrained by a river, providing a constant head boundary of 96 feet MSL in the northeast corner of the site and linearly decreasing to 95 feet MSL at the southeastern corner of the site. Both north-south boundaries were assumed to be no-flow boundaries. A second unknown disposal source was also present at the site. No information concerning this source was supplied to any of the evaluation testers before to the start of the investigation. If during the investigation they encountered the second plume, they were given the corresponding information for the location they were testing. Although this may appear unfair, it represents a common occurrence in site characterization efforts.

The results from the contaminant flow over the 15 years prior to the investigation were simulated using the USGS Method of Characteristics (MOC) code. Table 1 presents the modeling variables used to perform the simulation. As stated above, the hypotehtical contaminant is an LNAPL, which cannot be modeled with MOC and generally is a very difficult contaminant to model. To overcome this difficulty, it is assumed that modeling the aqueous phase is conservative and the problem can be treated in only two dimensions. The site was

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gridded into 240 nodes (20 in the east-west direction and 12 in the north-south direction) spaced every 200 feet in each
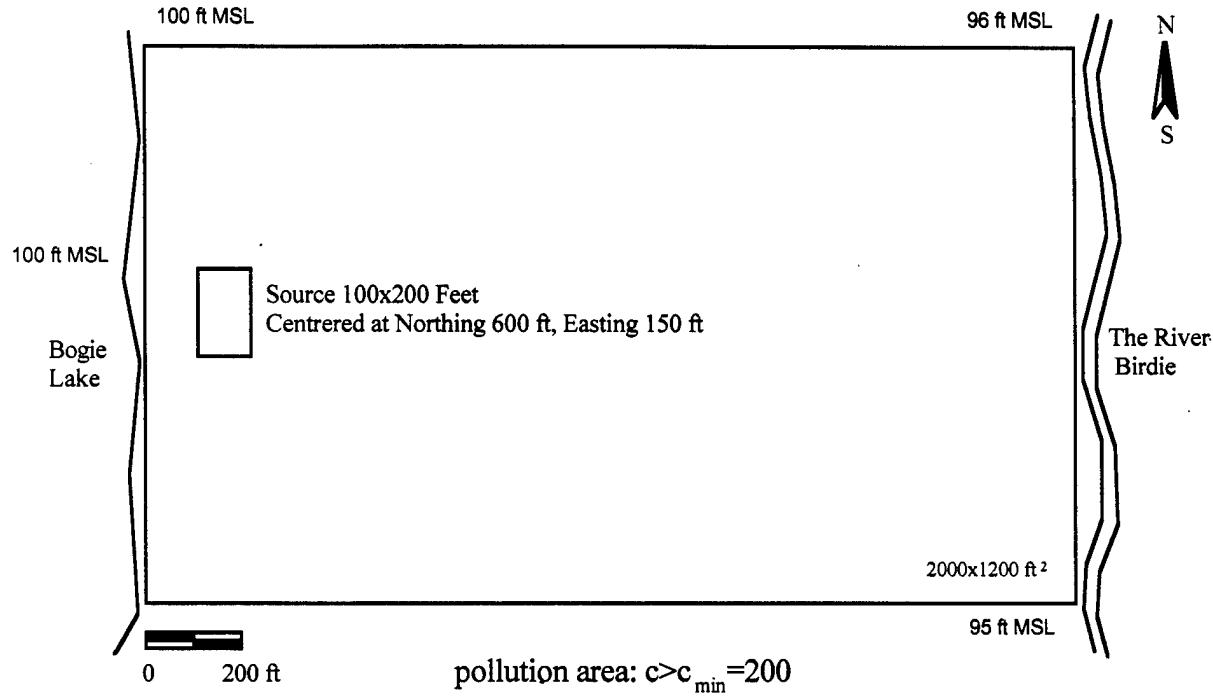

Figure 2.   Test Case Problem Definition.

TABLE 1. PARAMETERS FOR MOC SIMULATION.

VARIABLE			PARAMETER
GRID DESCRIPTORS			
NX	(NUMBER OF COLUMNS)	=	20
NY	(NUMBER OF ROWS)	=	12
XDEL	(X-DISTANCE IN FEET)	=	200.00
YDEL	(Y-DISTANCE IN FEET)	=	200.00
TIME PARAMETERS			
NTIM	(MAX NO. OF TIME STEPS)	=	15
NPMP	(NO. OF PUMPING PERIODS)	=	1
PINT	(PUMPING PERIOD IN YEARS	=	15.000
TIMX	(TIME INCREMENT MULTIPLIER)	=	0.00
TINIT	(INITIAL TIME STEP IN SEC.)	=	0.0
HYDROLOGIC AND CHEMICAL PARAMETERS			
S	(STORAGE COEFFICIENT)	=	0.000000
POROS	(EFFECTIVE POROSITY)	=	0.30
BETA	(LONGITUDINAL DISPERSIVITY)	=	20.0
DLTRAT	(RATIO OF TRANSVERSE TO LONGITUDINAL DISPERSIVITY)	=	0.40 = 8 FEET/DAY
ANFCTR	(RATIO OF T-YY TO T-XX)	=	1.000000
EXECUTION PARAMETERS			
NITP	(NO. OF ITERATION PARAMETERS)	=	7
TOL	(CONVERGENCE CRITERIA - ADIP)	=	0.10E-01
ITMAX	(MAX. NO. OF ITERATIONS - ADIP)	=	150
CELDIS	(MAX. CELL DISTANCE PER MOVE OF PARTICLES - M.0.C.)	=	0.500
NPMAX	(MAX. NO. OF PARTICLES)	=	5000
NPTPND	(NO. OF PARTICLES PER NODE)	=	9

direction. Nine particles per node were used to track the contaminant. Simulations took approximately 10 minutes on a 486 PC 66 MHz computer. The results from the final simulation were then contoured using the contouring package in UNCERT. The algorithm used by UNCERT consists of determining the equation of the plane between three points surrounding an intermediate point, and then solving that equation for either a given concentration value or a given location within that triangle. The contoured results are presented in Figure 3. This same algorithm was used to develop a computer code for calculating the contaminant concentration at any selected input point. This code was then used to determine the contaminant concentration at any location selected by either an engineer or a computer code. This allowed the users to conduct investigations using only the site map in Figure 2, along with only the results determined from their investigation.

C.   TRADITIONAL ENGINEERING PROCEDURES

The current state of practice and the approach taken most often consists of sampling a predetermined grid, returning from the field and then evaluating those results. This approach is highly ineffective and generally results in a return to the field for measurement of in-fill locations. The current state of the art consists of an engineer-guided investigation, using results from a real time method (such as Cone Penetrometer Testing) with real-time chemical sensor (such as Laser Induced Fluorescence). The baseline approach against which the I/A-Site system was evaluated was the current state of the art rather than the current state of practice.

Using this baseline, we asked three experienced engineers to evaluate our test case problem. Each engineer was given the site map with the soil type, hydraulic conditions, and the source location of the disposal pit. The objective of their study was to determine all soil regions with contamination levels above 200. They were asked to identify when they felt they had gathered enough samples to determine that they had located both 85 and 95 percent of the contamination. Each engineer was assisted by a computer program that informed the user of the concentration level at each tested location. This simulated the same information available if

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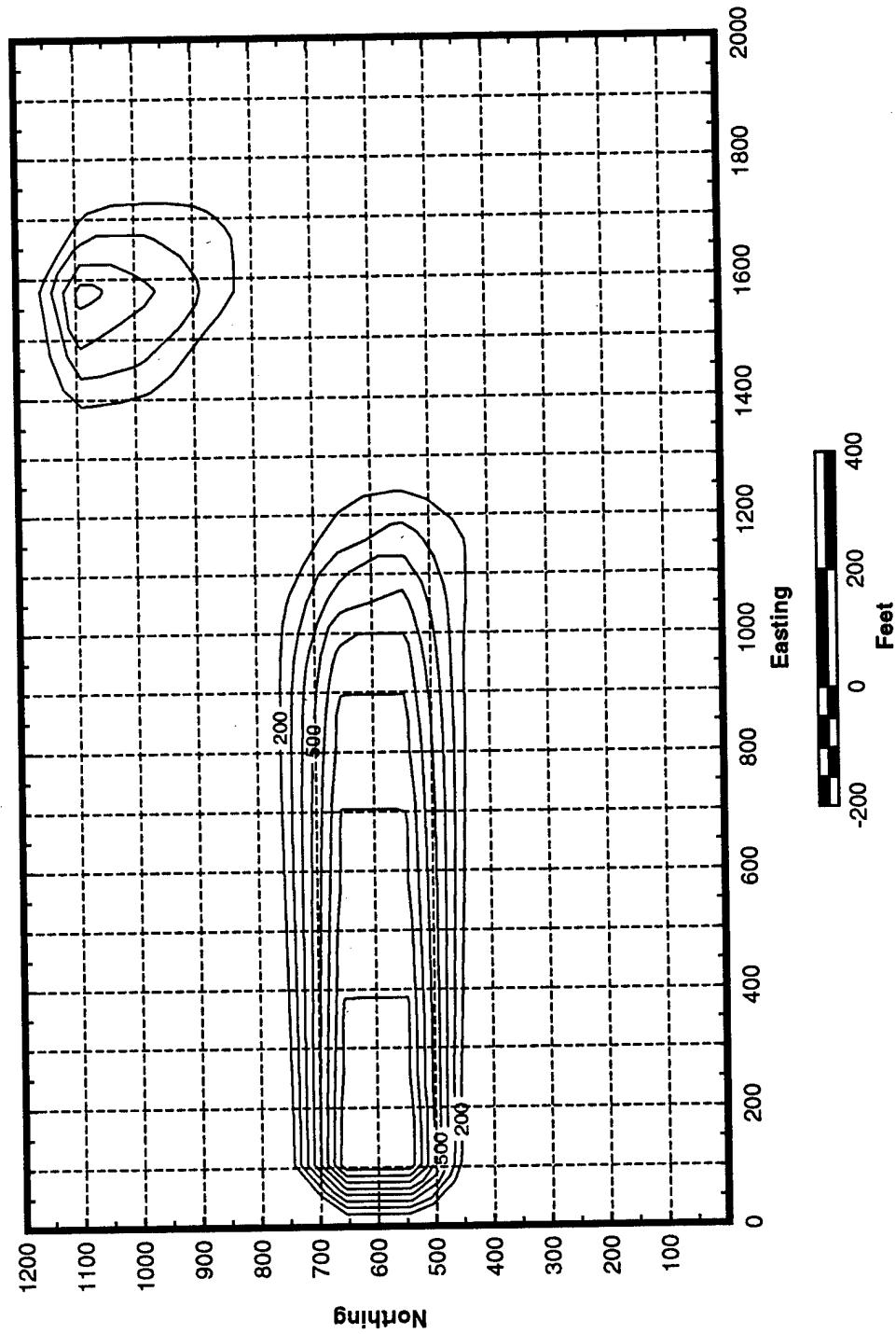
Figure 3. Contaminant Distribution for Test Case.

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conducting the investigation using a CPT testing methodology.

The results from the study were interesting, with the three engineers choosing from 15 to 23 test locations to establish an 85 percent confidence level. To establish a 95 percent confidence level, 18 to 27 locations were required. Table 2 presents the selected locations and order determined by each of the three evaluating engineers. The spread represents a change of 50 percent, indicating some variance in how these investigations may be conducted in the field.

Figures 4 through 6 present the contoured results from each of the engineering solutions, as compared with the generated solution presented in Figure 3. In each figure, each node identified with an "X" has been correctly identified as contaminated and those identified as an "⊗" are incorrectly identified as contaminated. Correctly identified clean locations are left blank, and incorrectly identified clean locations are identified with a "⊕".

Table 3 presents a summary of the statistics for the three engineering solutions. Engineer 1 identified 31 of the actual 30 contaminated nodes. Although the number indicates Engineer 1 did very well, the engineer identified too many contaminated noes in the main plume and completely missed the second unknown plume. This is shown in Figure 4 as compared to the actual test case. In terms of the actual comparison to the correct solution, the engineer misclassified only 17 individual nodes for a rating of 93 percent on the total number of nodes, (i.e. 240 - 17 = 223). Engineer 2 did nearly as well, identifying 29 contaminated nodes but totally missing the second plume and over-estimating the main plume (Figure 5). In terms of actual number correctly identified, 17 nodes were missed, leading to a rating of 93 percent. The third engineer was not as successful and determined 40 contaminated nodes. Again, the second plume was totally missed and the main plume was significantly overestimated (Figure 6). In terms of actual nodes classified correctly, Engineer 3 generated an overall rating of 89 percent, with 26 nodes incorrectly classified.

Another perhaps more meaningful method of analyzing the engineering results in terms of remediation costs is to classify the estimate at each node as one of three categories: Correct; a

TABLE 2. ENGINEER SELECTED LOCATIONS.

Location	Engineer 1			Engineer 2			Engineer 3		
	X	Y	Con.	X	Y	Con.	X	Y	Con.
1	550	165	1.0	1300	225	2.0	150	600	978.5
2	900	1045	.6	1800	75	0	300	600	937.5
3	600	300	6.0	650	450	151	600	600	839.0
4	300	600	937.0	800	400	94.5	1200	600	839.0
5	800	600	763.5	450	500	496	1300	600	94.5
6	1600	500	5.0	750	700	478.5	150	400	10.5
7	1150	550	353	700	550	805	150	475	260.25
8	1350	550	65	400	350	21.5	150	725	260.25
9	1250	450	81	400	350	5.5	600	375	42.5
10	1150	650	261	300	550	937	600	475	321.75
11	1200	600	210	300	450	60	600	775	110.75
12	950	450	176	300	800	39	600	725	321.75
13	500	500	510	950	600	661	900	700	417.0
14	650	700	488	1600	600	13.5	900	800	97.0
15	250	400	23	1200	600	500	1200	750	52.5
16	450	750	104	1200	600	210	350	762.5	67.0
17	75	600	245	300	725	288	350	725	287.0
18	5	600	ND	550	800	70.5	100	450	10.5
19	10	600	ND	50	600	0	90	490	8.40
20	25	600	ND	500	400	57	100	600	489.0
21	50	600	ND				95	600	440.1
22	800	400	95				75	600	244.5
23	925	725	294				50	600	0.0
24							900	425	137.5
25							1175	475	206.5
26							1250	600	141.0
27							475	425	85
28									

TABLE 3. SUMMARY STATISTICS.

|	Engineer 1	Engineer 2	Engineer 3	Averages
Contaminated Nodes	31	29	40	33
Clean Nodes	209	211	200	207
Correct Nodes	223	223	214	220
Incorrect nodes	17	17	26	20
Type 1 Errors	8	9	8	8
Type 2 Errors	9	8	18	12
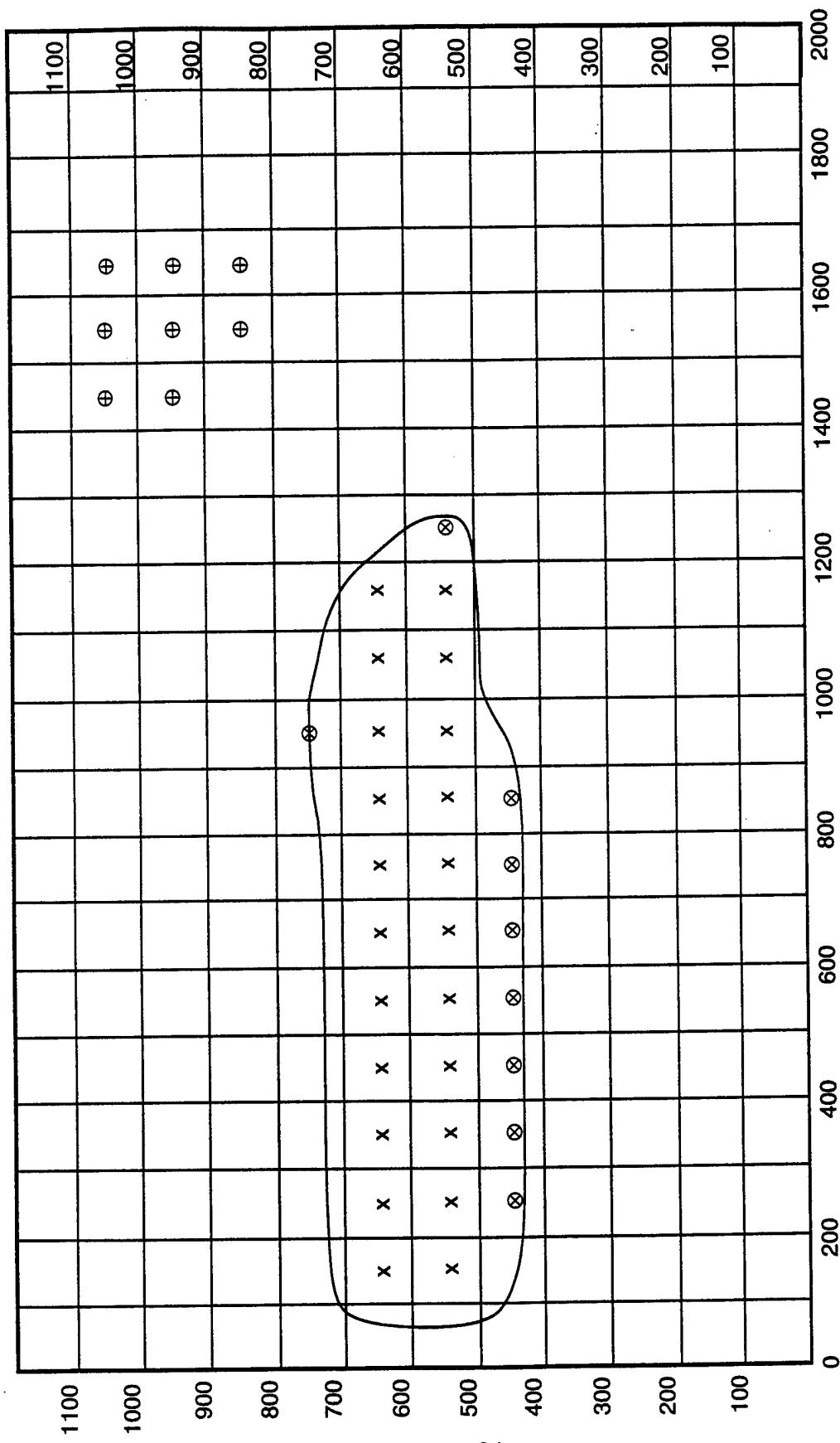
Figure 4. Contaminant Distribution for Engineer 1.

24
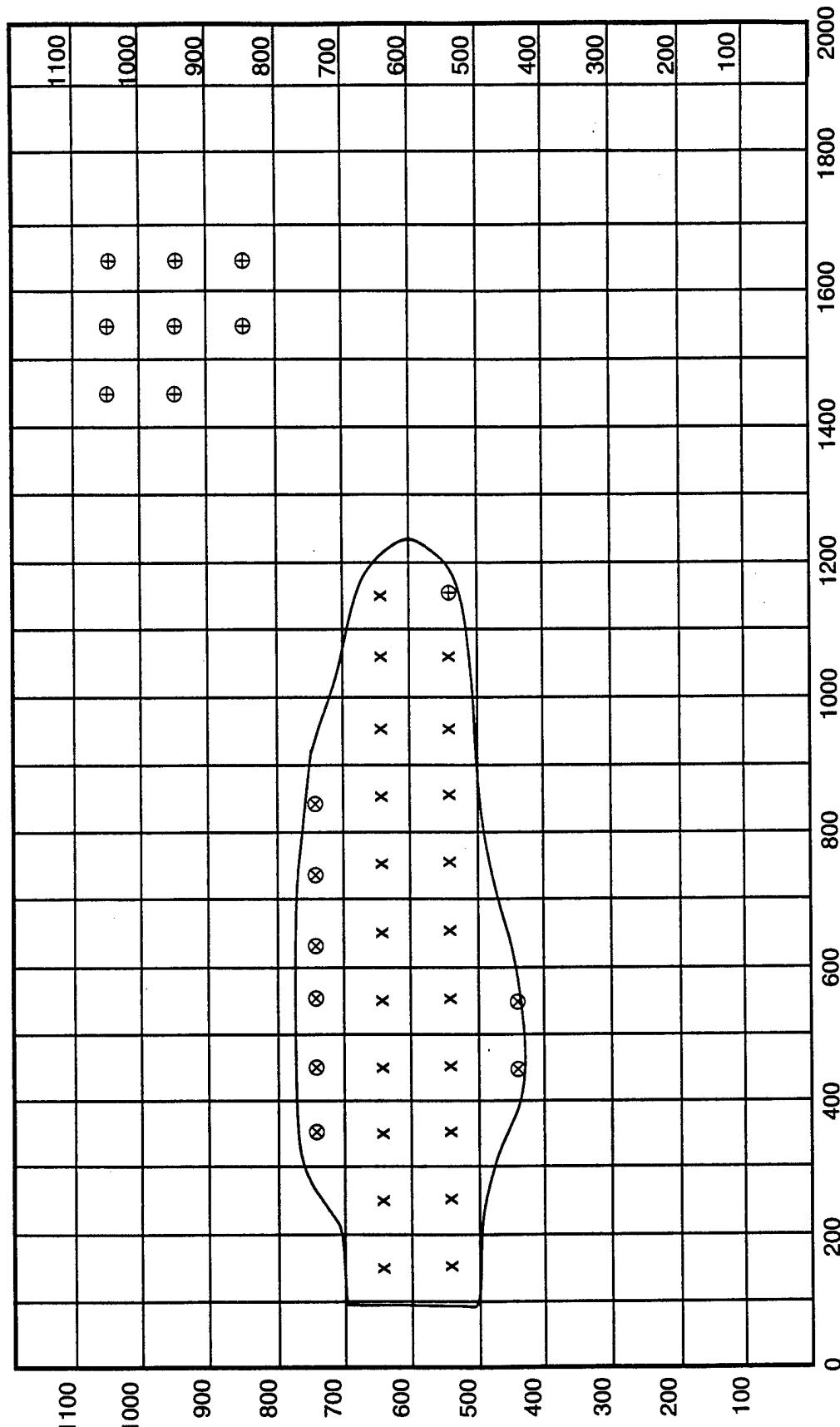
Figure 5. Contaminant Distribution for Engineer 2.
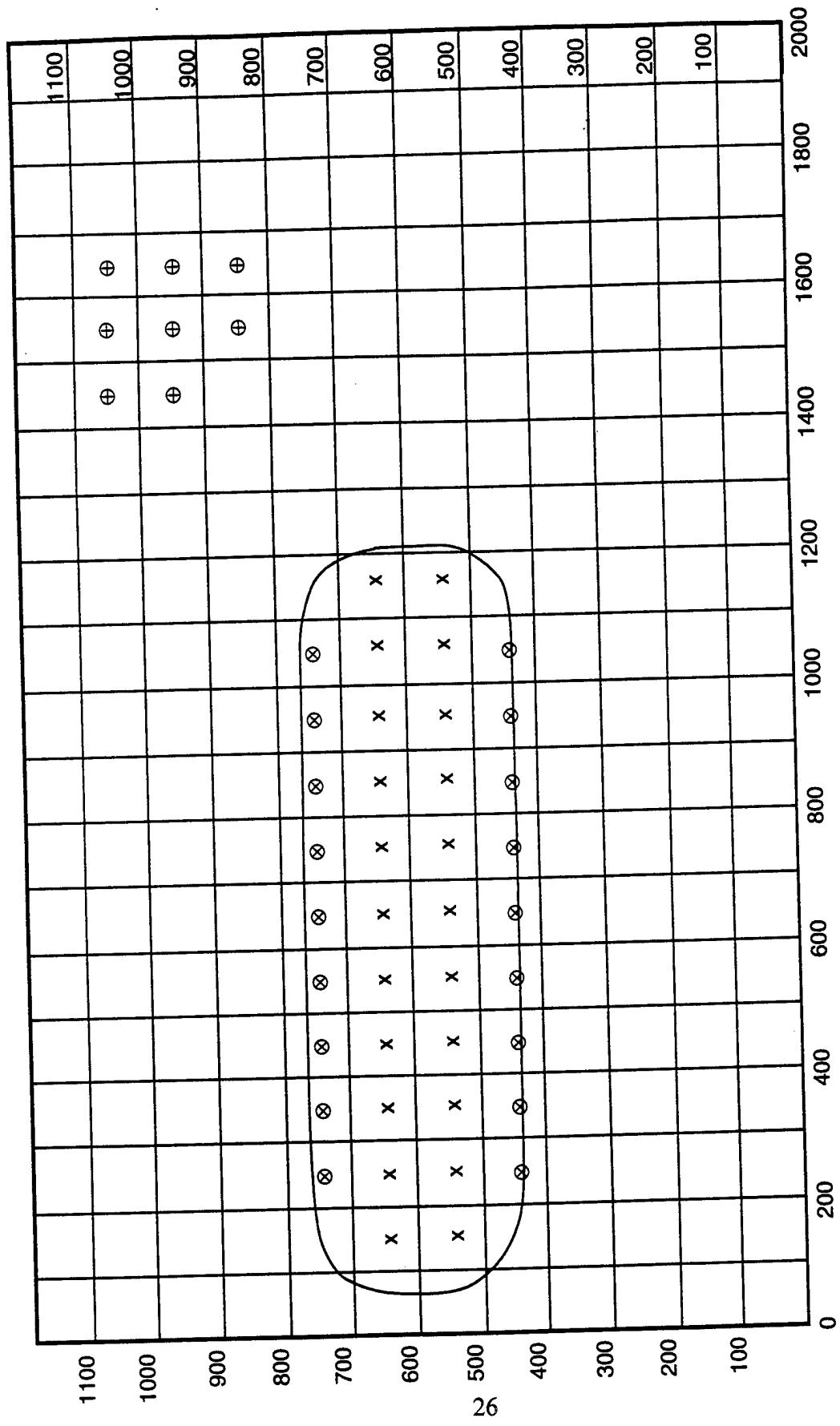
Figure 6. Contaminant Distribution for Engineer 3.

Type 1 error (i.e., identified as clean when actually contaminated); or a Type 2 error (i.e., identified as contaminated when actually clean). The two types of errors are significant when figuring the remediation costs because they are weighted differently. Typically, it is more costly to correct a non-remediated area and pay any penalties than to remediate a few zones not in need of remediation. This is not to say that it is better to remediate the entire site, but rather to err on the conservative side.

Based on this type of analysis, Engineer 1 committed eight Type 1 errors and nine Type 2 errors. Engineer 2 was roughly the same with nine Type 1 errors and eight Type 2 errors. Engineer 3 finished with eight Type 1 errors and eighteen Type 2 errors. In all cases, the number of Type 1 errors was very uniform, mostly due to all three engineers missing the second contamination region of eight contaminated nodes. The average number of Type 2 errors was twelve, indicating a trend of over-estimation of the contaminated zone.

Overall, the engineers' solutions were fairly consistent. The solution for Engineer 3 involved several more tested locations, but the average established a solid baseline that other methodologies can be compared with. Postanalysis discussions with Engineer 3 indicated that he was looking for a trick in the puzzle. The unknown source was not identified by any of the engineer s' solutions. Engineer 3 was most likely biased by the nature of the question, but his bias does not significantly affect the average.

D.   PLUME SOFTWARE CODE

PLUME is one of four codes implemented in the software package for both the selection of optimal sampling locations and assessment of the current level of uncertainty. PLUME accomplishes these two tasks by using a combination of Bayesian analysis and indicator spatial statistics. This approach provides a means of quantitatively integrating "soft" information (such as non-intrusive geophysical survey results, historical records, and past experience about the potential extent of contamination) with "hard" sampling data generated during previous site

characterization activities. It is this combination of hard and soft data that greatly assists the user during the initial stages of the site characterization process. In general, little if any hard data are available early in the site characterization process; therefore the process must rely upon the soft data. As the investigation continues, the hard data become more available and the utility of the soft data is reduced.

By integrating soft data, estimates of contaminated volumes are possible, along with the uncertainty levels associated with those locations. By analyzing the uncertainty functions, optimal sampling locations can be selected to reduce the uncertainty. The evaluation of new locations involves the assessment of the uncertainty reduction which can change as a result of the information gathered at each new sampling location. The uncertainty functions provide a measurement of whether the site characterization efforts have achieved the desired level of confidence required.

To accomplish these two goals, PLUME uses the concept of ordinary indicator kriging. Kriging not only provides interpolation estimates based upon sample data, but also estimates the error associated with those interpolations. A practical description of kriging in general can be found in Isaaks and Srivastava, 1989 (7). Ordinary kriging determines interpolated values by assigning optimal weights (w_i) to each sampled data point, $Z(x_i)$, to construct linearly interpolated values, $Z(x_o)$, as presented in Equation 1. The weights are "optimal" in the sense that they provide unbiased linear interpolations with minimum interpolation error.

$$Z(x_o) = \sum w_i \, Z(x_i) \qquad (1)$$

PLUME expands upon the concept of ordinary kriging by incorporating a Bayesian approach. The Bayesian approach differs from classical statistics by assuming that parameters of interest (such as the presence of contamination at a particular location) are unknown initially, but have some known probability distribution function (prior pdf). As additional information becomes available regarding the actual values of the parameters, Bayesian analysis provides a

quantitative method for merging the new information with the prior pdf to obtain what is known as the posterior pdf via Bayes rule.

$$P(x|y) = P(x)P(y|x) \qquad (2)$$

The final key aspect incorporated in the PLUME methodology is the concept of indicator kriging. Indicator kriging differs from kriging in that binary indicators (such as the presence or absence of contamination at a location) are used instead of parametric values (such as the concentration level at a location). A more detailed description of indicator kriging can be found in Journel, 1983 (8). One of several advantages of indicator kriging for this application is that indicator kriging relies upon a more robust estimated variogram than ordinary kriging, partly because it is immune to outlying sample values. Indicator kriging can also be applied to data that are only qualitative, such as data generated in many field screening applications. Also, indicator kriging makes no assumptions about the distribution of contamination or that the data set is stationary.

Using the PLUME code, two researchers evaluated our test problem. The first researcher was an inexperienced PLUME user, while our second researcher was the developer of PLUME. By comparing these results, we sought to learn if operator experience influenced on the obtained results. In both cases, the operators had to assume an initial probability distribution function. The novice user selected a probability of contamination of 50 percent over the entire site, except for the disposal pit, which was given a probability of 100 percent and a small region downstream of the pit, which was given an 80 percent probability of being contaminated. Our experienced user selected basically the same initial probability distribution function, except the regions upstream of 45 degree lines from the disposal to the site boundary were given a probability of 20 percent of being contaminated.

For each initial case, PLUME was operated to selected the next sampling location such that the regions of contamination are maximized. This mode of operation was continued for roughly 8 locations and then changed to maximize the clean regions. This mode was continued by

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each researcher until they felt the site had been characterized to a 95 percent confidence level. It should be noted that PLUME provides an estimate of the number of cells classified as uncertain given a specified confidence interval. The method PLUME uses to perform this calculation is to take the confidence interval (i.e., 90 percent) and assign all points with a probability of contamination of less than 0.1 as clean and all points with probabilities of greater than 0.9 as contaminated. All points with probabilities of contamination between 0.1 and 0.9 are classified as uncertain. Using this approach, significantly more penetrations are required to reduce the uncertainty category to zero at 90 percent confidence than the number of penetrations required for an engineer to reach a 90 percent confidence level. This is because PLUME uses statistics over the entire site, whereas the engineer is concerned with estimating only the region of contamination to a specified confidence level. Based upon this later approach, each of the operators ran the model until they were 90 percent confident they had identified the plume.

The novice operator characterized the site using PLUME in a total of 24 penetrations. Assuming probabilities greater than 75 percent were contaminated, a total of 5 cells were identified as contaminated after the 24 locations. Assuming all other cells as clean produces a total of 235 cells, or 213 cells correctly identified. This value compares with the 220 cells correctly identified by the engineers. In terms of the Type I and II errors, a total of twenty-six Type I errors were identified and one Type II error. These compare with eight Type I errors for the engineering solution, and twelve Type II errors for the engineers. If the concentration probability is decreased to 50 percent as a contaminated cell, then the Type I errors decrease to fourteen and the Type II errors increase to eight.

The results from the expert user were very similar. Of the 240 cells, 228 were identified as clean, using a 75 or higher percent probability as a contaminated cell. This produced 218 cells correctly identified, which is 5 cells higher than the novice user. Of the 22 cells misclassified, 20 were Type I errors and two were Type II errors. If the contamination probability is lowered to 50 percent, the experienced user had twelve Type I errors and nine Type II errors. Once again,

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this is similar to the novice user, indicating that user experience does not significantly influence the results.

E.   SCANN

The second easiest tool to use in the package is the Site Characterization Artificial Neural Network (SCANN) code developed by the University of Vermont. This code uses artificial neural networks to complete pattern recognition problems. The benefits of using SCANN are that it is data-driven and requires no estimate of the covariance function to begin operation. Given some fixed amount of information, SCANN uses a feed-forward counter-propagation training approach to determine a "best estimate" or map of a discrete spatially-distributed field. The method can readily be applied to one-, two-, and three-dimensional mappings and can be used as part of a conditional simulation approach. The combination of simplicity and computation speed make SCANN ideally suited for a variety of characterization problems.

To demonstrate some of its utility, SCANN was used to evaluate the test problem. Since SCANN is not able to predict penetration locations, it can not solve the entire problem; but it can be used to effectively map the results after a given number of holes, and based upon that data, estimate values for untested locations. To demonstrate this, the results from the first 14 penetrations of Engineer 1's solution were used to train the network in order to make predictions over the entire site. Since SCANN operates only on categorized values rather than real values, the results were categorized as clean or contaminated based upon a concentration value of 200. Figure 7 presents the output from the network for the entire site. In comparison with Figure 3, the SCANN map resembles the correct solution and does indicate potential contamination at the location of the second plume. The region of the main plume is significantly larger in the SCANN map, especially on the upgradient side. This is most likely due to the lack of data upgradient to the disposal site. Another interesting note is that, based upon the limited data, SCANN attempted to connect the two plumes, and therefore tended to misclassify those points in the

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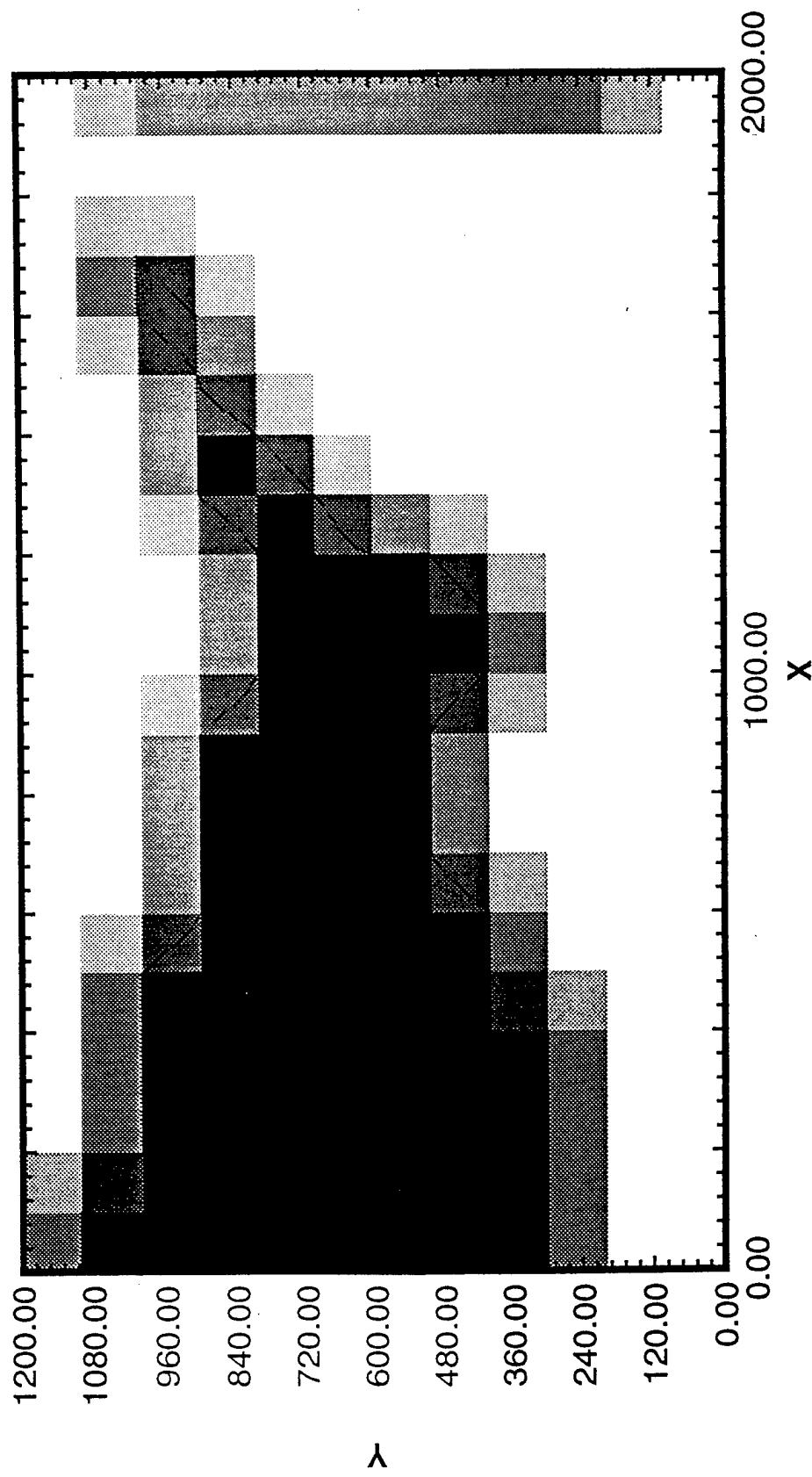
Figure 7. SCANN Output with Two Categories: Clean and Contaminated.

32
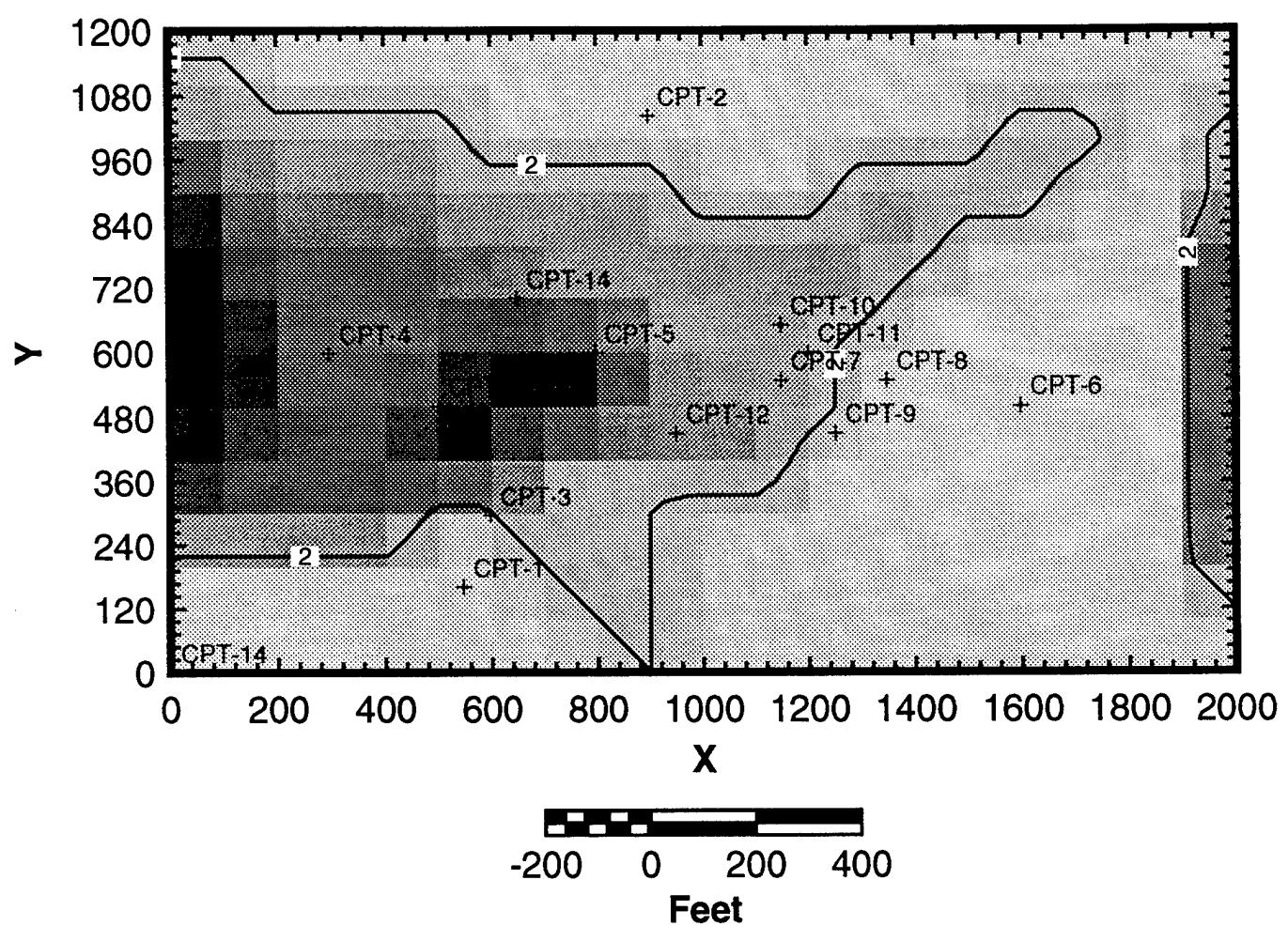
Figure 8. SCANN Output with 10 Categories.

middle. Of the 240 cells, a total of four were Type I and forty-two were Type II errors. This was significantly lower in terms of Type I errors, but higher in terms of Type II errors. The statistics from the engineering solutions were based upon approximately 20 data points and SCANN was operated using only fourteen data points.

This approach demonstrates the ability of SCANN to provide binary maps of hits and misses. To further demonstrate SCANN's mapping capabilities, we have also solved the same problem using ten categories rather than two. The categories were assigned as "1" for concentrations between 0 and 100, "2" for 101 to 200, "3" for 201 to 300, and soon, up to "10" for concentrations between 901 and 1,000. Using these ten categories, the network was retrained and the output presented in Figure 8. As expected, this figure has much more detail than the previous model. Once again, accuracy near the edges is questionable due to the lack of data in these regions.

As presented, SCANN can be an easy-to-use part of the site characterization process. All that is required of the use is the entry of the training data set and the selection of the desired output grid. For the sample problems the run portion of the code took under one minute on the developed system. This speed allows the code to be used often, i.e., retrained after each location or as part of a statistical simulation program. A part of the code not demonstrated here but which could be of use for location selection is the confidence index that is provided for each output point. This value is an indicator of the certainty of the given category's validity. Using this value, potential error maps could be generated and used to guide the engineers selection of the next location.

F.   EXAMPLE OF OSCAR - COST ANALYSIS CODE

A key part of the site characterization process is the ability to decide when sufficient sampling has occurred and the site is appropriately characterized. As part of this determination of an appropriate level, it must be decided if the costs of additional sampling outweigh the cost
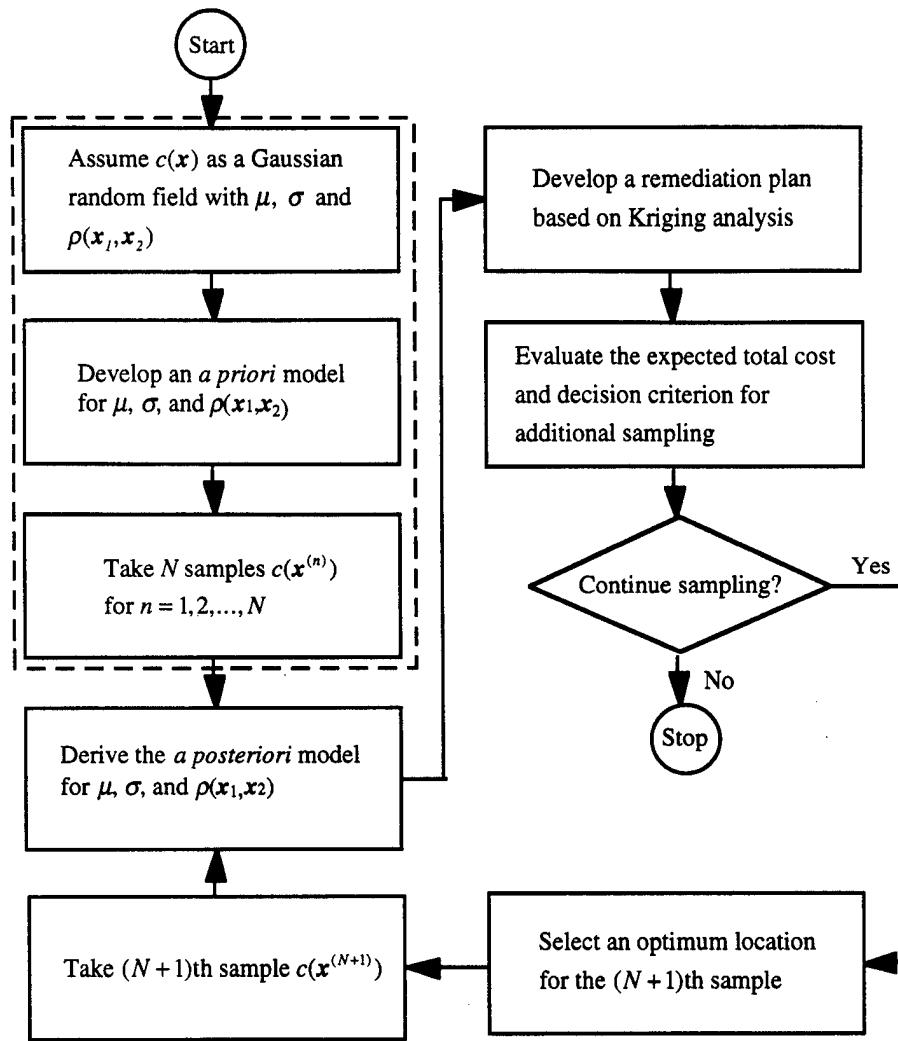
Figure 9.   Decision Analysis Flowchart for Adaptive Sampling.

reduction which may occur as a result of this additional information. To assist the user in making these decisions, ARA has developed a code called Optimal Site Characterization and Remediation (OSCAR).

OSCAR includes a quantitative methodology for assessing the reliability of the current remediation plan and determining the need for additional samples. This information provides the basis for formal optimization of sampling strategies and remediation plans. The logic incorporated into the code is presented in Figure 9. The simple cost function used in the development includes a penalty cost for failing to remediate contaminated area and unnecessarily remediating clean areas. The utility of the code is but illustrated through the use of an example.

The example that will be used is the same test case as presented previously. The cost per sample is assumed to be $500, the cost for remediating each element (i.e., the area centered around a node) is $2,500, and the cost associated with failing to clean up a contaminated element (i.e., a "false negative") is $10,000. An element is considered to require remediation if its contaminant level at the node exceeds 200 units, as shown on the contour plot of Figure 3. All samples are assumed to be exact (i.e., sensor error is neglected). The objective is to determine the contaminant plume boundary and develop a remediation plan. The secondary plume in the northeast quadrant is the result of an unidentified contaminant source. It is included in the example problem to test the ability of the methodology to discover unsuspected secondary plumes.

Figure 10(a) presents the location of the first 12 sampling points. Based on this information, the random field properties are estimated with mean 331 and standard deviation 302. The correlation length cannot be estimated from the data alone because the number of samples is too low; hence, it is assumed to be 400 feet (based on previous experience with similar site characterization problems). Using simple kriging (SK), the predicted contaminant concentration and associated variability are obtained and shown in Figure 10 (a) and (b), respectively. Notice how the standard deviation increases away from the sampled points.

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Cleaning up the site based on the SK predicted contaminant concentration will cost $265,000 (106 contaminated elements @ $2,500 per element), however, because of the relatively small number of samples there is large uncertainty associated with the SK prediction. Using the Monte Carlo simulator in OSCAR, the expected number of false negatives (i.e., the expected number of contaminated elements that are missed and left untreated) is 16.165, and the cost is $161,650 (16.165 missed elements @ $10,00 per element). Given that sampling is relatively inexpensive ($500/sample) and the potential returns are great (i.e., potential for uncertainty reduction), and the expected cost of false negatives is high, we opt to continue sampling.

Table 4 lists the costs associated with continued sampling at the site. At each stage, OSCAR is again run to assist in the decision to continue sampling. Figure 11 illustrates that as the number of samples increases, the uncertainty in the total cost generally decreases but not monotonically. There are two reasons for fluctuations. First, the mean and standard deviation of the random field can change dramatically as additional critical samples are included. This is typical when the number of samples is small. For example, samples 15 and 18 dramatically reduced the expected cost of false negatives by taking concentration data in highly uncertain regions of the site. Sample 22 reduces the expected remediation cost by $25,000 by identifying

TABLE 4. OPTIMAL SITE CHARACTERIZATION EXAMPLE RESULTS

| Samples	Cost for Cleanup ($)	Expected Cost for False Neg. Id. ($)	Expected Total Cost ($)	COV_{total}
12	265,000	161,650	432,650	0.21
13	247,500	156,300	410,300	0.22
14	200,000	201,500	408,500	0.24
15	180,000	164,850	352,350	0.25
16	170,000	158,700	336,700	0.28
17	167,500	141,900	317,900	0.29
18	165,000	94,350	268,350	0.22
19	165,000	95,400	269,900	0.21
20	177,500	90,649	278,150	0.18
21	195,000	70,100	275,600	0.17
22	170,000	80,800	261,800	0.19
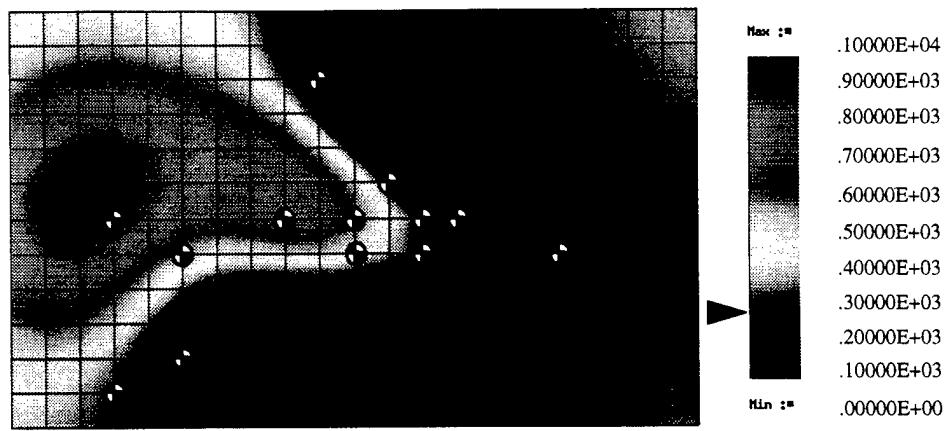
(a)
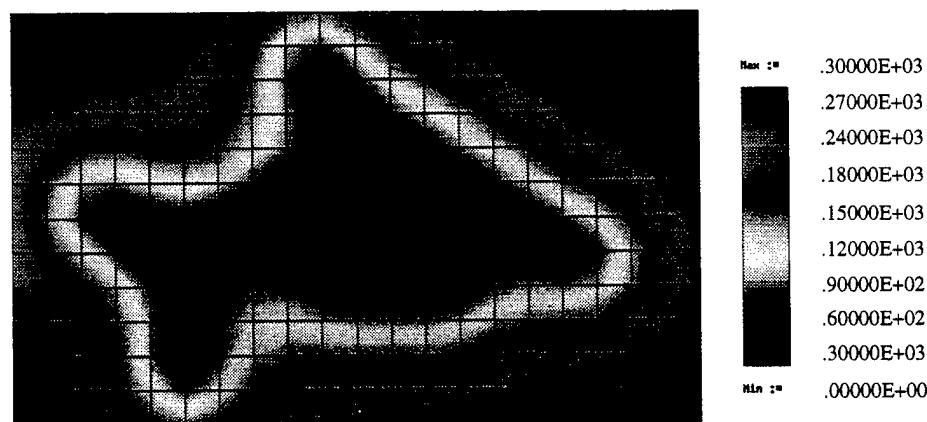
(b)

Figure 10. Prediction Based on 12 Samples.
(a) Predicted Contaminant
(b) Associates Standard Deviation
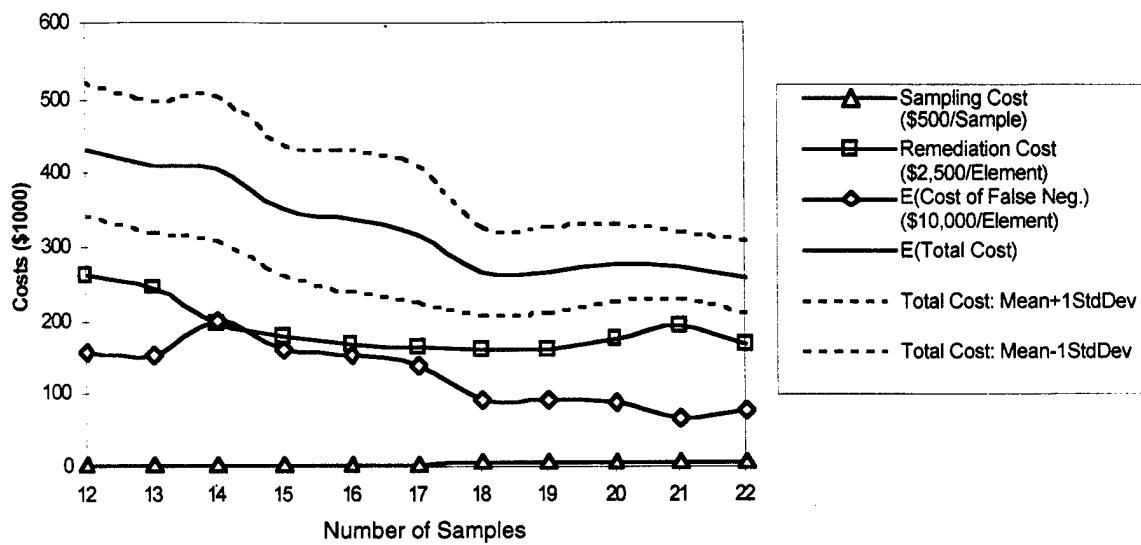
(a) Baseline Unit Costs
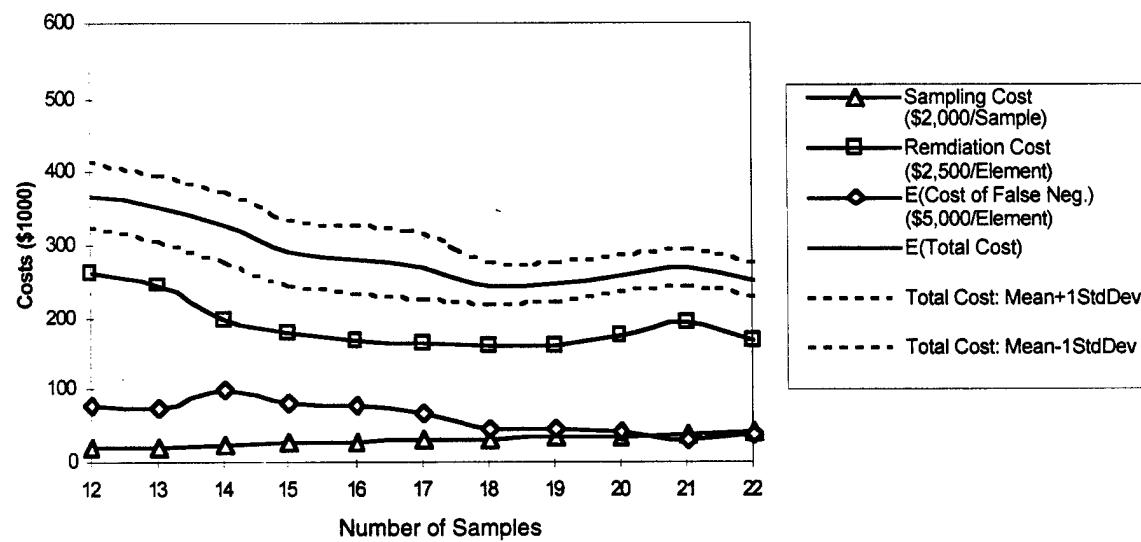
(b) Sample Excursion for Unit Costs

Figure 11.   Cost Curves for Site Characterization Sample Problem

the boundary of the secondary plume. Second, the costs for false negatives and false positives are different, so when additional samples are included, the number of false negative elements may increase even though the total number of false identifications decreases. These fluctuations will stabilize as the number of samples increases.

The cost of obtaining the 22 samples represents less than 5% of the expected total cleanup cost; thus, there is little incentive to cease sampling at this point. If, however, sampling costs were higher (e.g., $2,000 per sample instead of $500 per sample) and the cost of false negatives were lower (e.g., $5000 per element instead of $10,000 per element), the cost curves would be as shown in Figure 11(b). In this case, the expected cost of false negatives has fallen below the sampling cost after 21 samples, and the total cost and its uncertainty are relatively stable after 18 samples. In this case, the costs of further sampling are likely to outweigh any further reductions in the expected cost of false negatives; therefore, sampling should be terminated for this case.

SECTION IV

SUMMARY AND RECOMMENDATIONS

A.   SUMMARY

A research program was conducted to develop a computer analysis system to assist field personnel conducting environmental site characterization projects. The goal of the project was to develop a user-friendly software system which could be used to analyze field data in near real-time and to select additional sampling points based on the prior data set. The software package, entitled I/A-Site (Intelligent/Adaptive-Site Characterization) is designed to run on a high-end IBM compatible PC with a minimum of 32 Megabytes of memory and one gigabyte of hard disk space. As of the date of the project, many of the available geostatistical codes and environmental site characterization database programs only run on the UNIX operating system, hence the PC computer is set up to operate under both UNIX or Windows operating systems.

The I/A-Site software package is designed to be modular so that additional analysis or graphics programs can be added as desired. Major software components of I/A-Site include: (1) SitePlanner® from ConSolve, which serves as the data base, links the various software packages and provides 2-D graphics capability; (2) ConeTap from ARA, which analyzes CPT data and provides the data in a format compatible for use by I/A-Site, and (3) three geostatistical codes (PLUME developed by Argonne National Laboratory, SCANN developed by the University of Vermont, and UNCERT, developed by the Colorado School of Mines). A probabilistic groundwater flow code, POWDER, developed by UVM is also provided, as is the 3-D graphics program SiteView developed by ConSolve. The final software code provided is OSCAR, developed by ARA which is a cost optimization program to determine when sufficient site characterization data has been collected. The software packages can be addressed in an X-Windows environment and data from a variety of formats (i.e. Excel spreadsheets, etc.) can be imported or exported.

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The IASite software system can take all current knowledge concerning a site and graphically display this data. The system extends further than data visualization with the incorporation of a variety of tools to assist the engineer in selecting optimal test locations and making informed decisions concerning further testing activities. Furthermore the software will assist the engineer in determining if the costs of additional testing are justified while considering total cleanup costs and the accuracy levels required. The use of these types of tools facilitates more effective site characterization. Capabilities which have been incorporated into the IASite software include:

- The ability to store and recall a diverse data set, including analytical results, drilling logs, geologic descriptions, results from geophysical testing etc.

- A simple to use graphic system to develop overlay plots of the diverse data set to show trends in the data and correlations.

- The ability to analyze and display the massive amounts of CPT data in order to determine important soil information.

- Geostatistical methods to develop maps of interest parameters, such as soil stratigraphy, water table surface, plume boundaries and concentrations, and the uncertainties of these properties.

- Decision analysis tools to assist field personnel in the selection of new test locations, the types of data to be obtained and the value of the additional data.

- A groundwater flow and transport model to assist in estimates of likely contaminate flow patterns, plume location and shape.

- Three-dimensional graphics system for use in the analysis of plume shape and presentation of results.

The cost of the IASite system was kept relatively low through the use of public domain and commercially available software. Total cost to Armstrong Laboratory to duplicate the system is approximately $17,500 plus the cost of a computer. The bulk of this cost is in the SitePlanner® database and graphics package and in the SCO UNIX operating system. These two

components cost approximately $14,500. The UNCERT analysis system is in the public domain and the project funded the development of the SCANN, POWDER and OSCAR codes. The remaining $3,000 cost is in the MT3D transport simulator, ConSolve's SiteView software and Applied Research Associates, Inc.'s Cone Test Analysis Program (ConeTap).

B.   RECOMMENDATIONS

At the time when IASite was developed, significant software limitations existed on the PC platform. These included lack of a multitasking operating system, limited number of geostatistical and 3-D graphics software packages and relatively slow performance as compared to workstations. In addition, the only user friendly graphical software package available on a PC was SitePlanner® from ConSolve, which required a UNIX operating system on the PC. Due to these limitations, it was necessary to develop some of the software using a UNIX operating system and a portion with the Windows operating system. To transfer data between codes developed on the different operating systems requires rebooting of the operating system. Dynamic data exchanges between the software packages was not possible, hence the user can not easily switch between the database and 3-D graphics program without rebooting. Since the project completion, Windows 95 has been released which solves many of the limitations of the Windows operating system. In addition, inexpensive Graphical Information System packages have been developed for the PC which can replace the UNIX based SitePlanner® graphical data based program.

Due to these changes it is recommended that the IASite program be converted to Windows 95 and incorporate a Windows based GIS database program and to fully integrate all of the software programs as 32 bit application. This will increase the speed of the analysis programs.

An additional recommendation is that the software be tested under field conditions and modified as required. This phase of the software development program was eliminated from the

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original program and IASite has not been fully evaluated in the field. The cost simulation model incorporated in the system represents an initial simple model, and additional models should be evaluated. These models could incorporate more complex penalty costs and also consider concepts of risk-based use issues.

SECTION V

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APPENDIX A

INTELLIGENT/ADAPTIVE SITE CHARACTERIZATION SYSTEM
USER'S MANUAL

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SECTION I
INTRODUCTION

A. OVERVIEW

The Intelligent/Adaptive Site (I/A-Site) Characterization system was developed to aid the engineer or hydrogeologist in site characterization. The system consists of a collection of software tools to perform database, visualization, geostatistical modeling, and data analysis functions. Each of the software tools in I/A-Site is discussed briefly in the next paragraph and later in this appendix. These tools are a collection of commercial and public domain software, all of which are copyrighted and their use, duplication, or disclosure are subject to restrictions stated in Contract No. F08635-93-C-0020 with Applied Research Associates.

The I/A-Site system has been tailored to allow easy import of field data into SitePlanner™, an object oriented database and visualization tool. Data can be visualized with plan views, cross sections and fence diagrams. Selected data can then be exported to the other programs for analysis. Xess™ is a general UNIX spreadsheet application through which SitePlanner™ imports and exports data. PLUME is a tool based on Bayesian indicator kriging used to select the next sample location. UNCERT is a collection of geostatistical tools for analysis of field data, modeling and visualization. MT3D is used in conjunction with MODFLOW for three dimensional flow and transport modeling. SCANN is an artificial neural network (ANN) program for interpolating field data. POWDER and PLUME are geostatistical tools to help the engineer predict the best location to sample next, and OSCAR is another geostatistical tool that helps determine the economic benefit of the next sample location before the sample is collected.

Section II of this User's Guide contains an introduction to X-Windows/Motif written by William Wingle and included in his UNCERT User's Guide (1). This section will help the user get familiar with most of the User Interfaces in the I/A-Site System. Section III is an overview of I/A-Site's main menu. This section briefly explains how each

of the programs is started. Section IV discusses the programs in more detail, how to run the programs from the I/A-Site and what additional documentation is available.

B.   DOCUMENTATION

Because the system is a collection of different software packages, (some commercial and some public domain), the system user's manual is a collection of the individual program manuals. This appendix contains a brief program description and instructions on how to start each program from the I/A-Site system. Detailed user's manuals for the commercial and public domain codes are contained in separate documents.

C.   HARDWARE AND OPERATING SYSTEM

The operating system for I/A-Site version 1.0 SCO system is Santa Cruse Operations (SCO) UNIX Release 3.0. The hardware which I/A-Site is currently operating on is a Pentium 60- MHz Intel processor with 40 Megabytes of Ram and a 1.2 gigabyte hard drive.

SECTION II
INTRODUCTION TO X WINDOWS/MOTIF[1]

Motif is an extension of the X-windows window manager interface. It provides a visually pleasing interface and allows the programmer to easily generate user-friendly features, such as push buttons, scrolled text windows, and pop-up dialogs. This section presents a brief overview of using Motif. Motif structures are used in I/A-Site User Interfaces. Once the user becomes accustomed to one module, other modules will also feel familiar.

A.   THE APPLICATION WINDOW

The application window is composed of six main components: 1) the application area, 2) the control button, 3) the title and movement bar, 4) the icon button, 5) the maximize and minimize button, and 6) the resizing bars and corners. These components are each shown in Figure A-1. The buttons and bars are activated by using the mouse pointer and pressing the left mouse button when the desired object is identified.

The application area refers to the area of the screen where the program is displayed.

The control button, when activated, displays a menu of window control options. However, most of the options can be more easily controlled by the methods discussed below. The one exception is the item "Close." Sometimes a window can "lock-up" and the application in the window no longer responds to the user. By selecting the "Close" menu option, X-windows destroys the window and terminates the application process. This is _not_ the recommended way to quit an application, but it is a reasonable approach when the application is no longer responding.

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[1] The Introduction to X WIndows/Motif was written by William Wingle of the Colorado School of Mines and was extracted from the UNCERT Users Manual.

B.   PULL-DOWN MENUS

All of the programs in the I/A-Site package are controlled by pull-down menus off the main menu bar. To activate a menu selection, point at the desired item on the menu bar and hold the left mouse button down. When the item is selected a pull-down menu will appear. While holding the mouse button down, point to the desired item and then release the button. Note that the currently selected item appears raised (Figure A-2). Moving the mouse point off all the menus and releasing the button unselects items. Some pull-down menu items have further options; these are identified by a small arrow to the right of the selection (i.e. "Type" in Figure A-2). When the user selects such an item, another pull-down menu is displayed.

Window Title

Title Box /
Move Bar

Icon Box

Window Control
Box

Maximize/Minimize
Box

Application Window

Window Resizing Bars/Corners
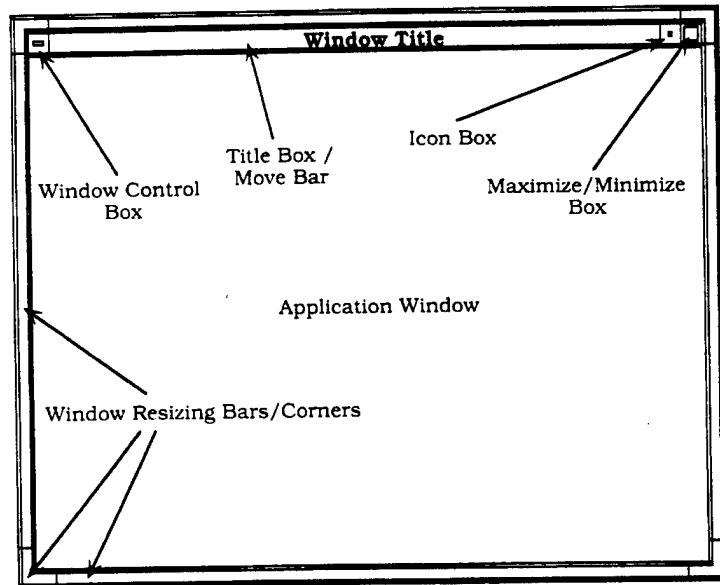
Figure A-1   X-windows/Motif application window components.
Besides the controls of a program application itself, the window manager allows the user to customize several aspects of the application interactively. Using window components, the window can be resized, moved, iconized, and destroyed.

It is also possible to use the menu without the mouse but by using keyboard commands. As shown in Figure A-2, most menu items have one character underlined. The underlined character identifies the key stroke that will activate each selection. Items on

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the main menu bar are selected by holding the <ALT> key with the appropriate character. Items from sub-menus are selected by typing the character only. For example, to select the GRIDZO file type, as shown in Figure A-2, the correct key stroke sequence is:

<ALT>F T G

For the rest of this manual, a menu-naming convention will be used. For this example, the text would refer to the menu item as *File:Type:GRIDZO*.

Some sub-menu items also have ellipses or "..." following them. This indicates that a pop-up dialog window will be displayed after its selection.
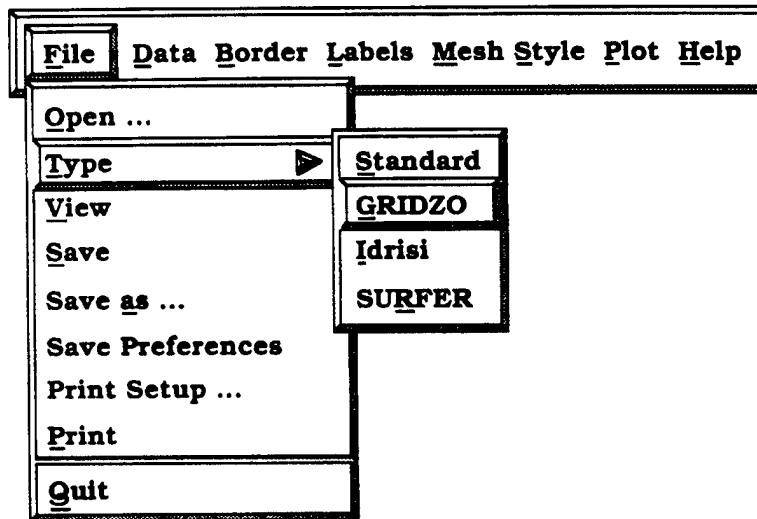
Figure A-2   X-windows/Motif pull-down menu.

This is a typical menu structure for an UNCERT program module, with the main menu-bar, the pull-down menu, and the sub-pull-down menu. The active selection is highlighted, by appearing as the most forward raised button. Note the underlined characters: these are "hot-keys" which allow the user to select most menu items using key strokes alone.

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C. POP-UP DIALOGS

A pop-up dialog is a temporary window created by the application. It is used to request information from or deliver a message to the user. The general format of a dialog window is shown in Figure A-3. In the *Dialog Response Area* there may be a series of buttons, text, text fields, scrolled text, slider bars, toggles, and toggle menus (each to be discussed). Below the response area are one to four buttons. (Figure A-3 shows *OK*, *Apply*, and *Cancel*. *Help* is also a commonly used button). The *OK* button is used to accept all the values defined in the dialog response area and remove the dialog. The *Apply* button also accepts all the values defined in the dialog response area, but the pop-up dialog is not removed. This option is often used in graphics programs to visually check how the graphic is modified by the parameter modifications before the dialog is removed. *Cancel* removes the dialog, and tries to discard changes made to values in the dialog response area. If *Apply* has been pressed, modified values cannot be canceled. If a <RETURN> has been used in a text field, the value cannot be canceled. Also, once a slider bar has been moved, its value cannot be canceled.

A simple dialog box may be composed of a message, and an *OK* button. Generally the message will inform the user that some other task must be performed before the desired selection will be executed, or that the application does not currently support that feature. After the user has read the message, pressing the *OK* button or hitting <RETURN> will remove the *Message* dialog.
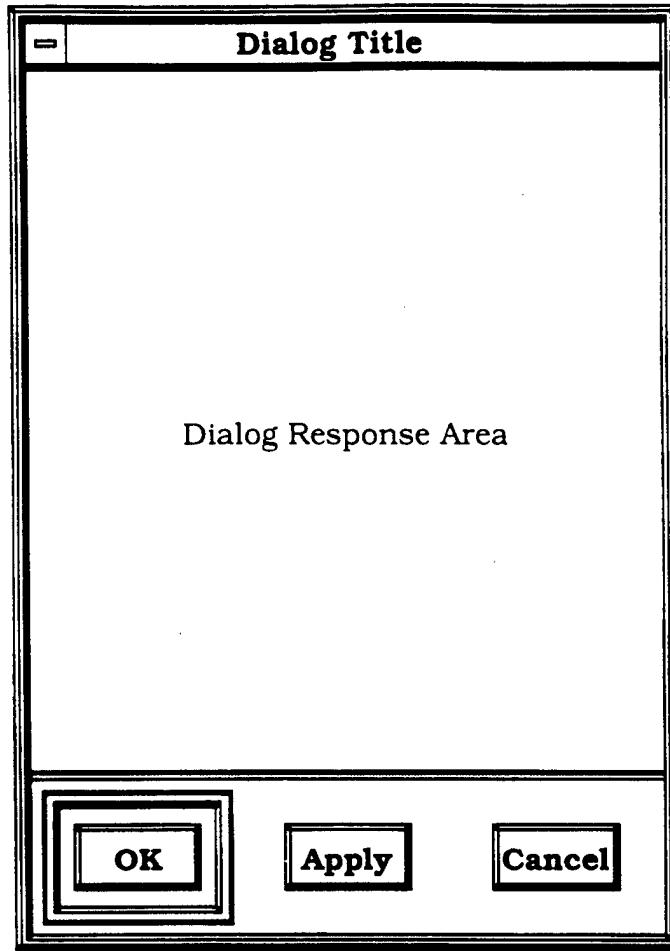
Figure A-3   X-windows/Motif pop-up dialog.
A dialog window is similar to an application window except that it cannot be iconized, and most pop-up dialogs (as the one shown here), as used in I/A-Site modules, cannot be resized. Pop-up dialogs, also always remain in front of the application, and when the application is iconized, the dialog is also hidden.

D.   BUTTONS:

Buttons are used to respond to a question, or request further information. As seen in Figure A-3, *OK*, *Apply*, and *Cancel* are responding to an implied question for the dialog: *"Are you done with the dialog and do you want the values saved?"*. If a *Help* button is

present, pressing it indicates information is desired about options in the pop-up dialog. The format of buttons is shown in Figure A-4. Buttons contain a text description and appear raised when they are available for selection. They appear recessed when they are activated.

Buttons may also be deactivated by the program. Often the function of a button becomes inappropriate due to the definition of other program inputs. By deactivating the button, the system does not allow the user to perform illegal operations or to supply more information then required. A deactivated button appears as a normal button, but the text descriptor is faded (Figure A-4).

| Push Button | Push Button | Push Button |

Figure A-4 X-windows/Motif push buttons.
As shown here push buttons have three main states: active, pressed and selected, and inactive, respectively from left to right.

E. SCROLLED TEXT:

Scrolled text areas are used to display textual information (such as a file) or to display a list of selectable user options (such as a list of all the files in the current directory). Often there is more information available then can be presented in the area supplied. When this occurs, scroll-bars are attached to the bottom and side of the text area (Figure A-5).

In the middle of the scroll-bar is a black button and at the ends are two arrows. If the black button extends from arrow to arrow, all the text is visible with regards to that scroll-bar. (The horizontal scroll-bar controls visible columns, the vertical scroll-bar controls visible rows or lines.) To move the view area one line or column at a time, press the appropriate scroll-bar arrow with the mouse pointer. To page down, press the gray area immediately below the scroll-bar button. To page up, press the gray area immediately above the scroll-bar button. A similar logic applies to the horizontal scroll-bar. Text can

also be scrolled by pressing the appropriate scroll-bar button, holding the mouse button, and dragging the button up and down (or left and right) as desired.

If the text field is a selection area, as with a *File Selection Dialog* (to be discussed below), the user may select the desired item by pointing at the appropriate line with the mouse pointer and pressing the left mouse button. This highlights the selected item. Note: Many programs allow double-clicking with the mouse on the selected item to execute the dialog's function (e.g., in a *File Selection Dialog* (to be discussed below), the user may select the desired item by pointing at the appropriate line with the mouse pointer and pressing the left mouse button. This highlights the selected item to execute the dialog's function (e.g., in a File Selection Dialog, double-clicking on a filename highlights the selection and passes the filename back to the program for further processing.)
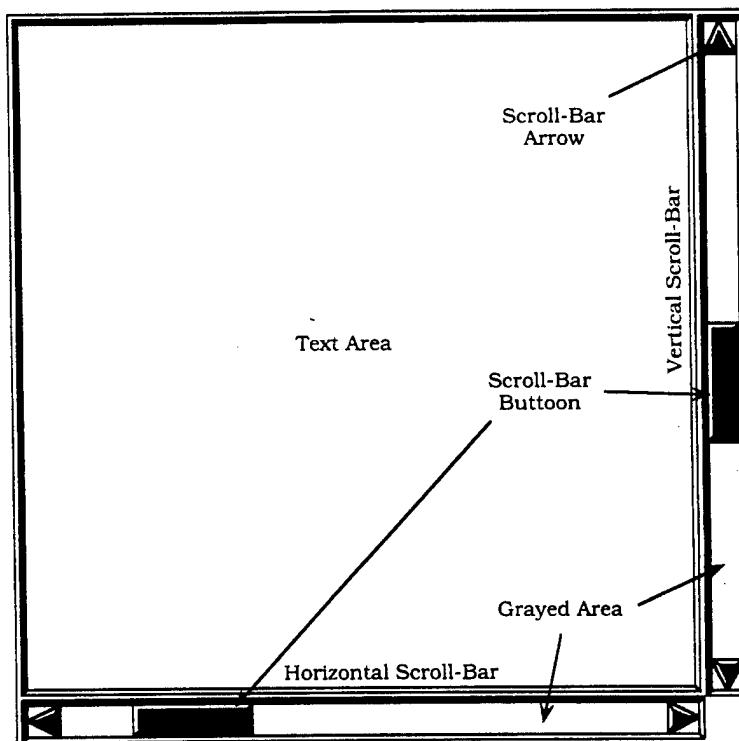
Figure A-5   X-windows/Motif   scrolled text window.

The scrolled text window is useful for examining long or wide test fields that will not fit completely on the screen.. The text is displayed in the text area, and if appropriate, the window will allow the user to scroll vertically and horizontally.

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F. SLIDER BAR:

A slider-bar allows the user to select a value from a closed range of continuous values. For example, the user may want to select a view direction over a surface. Because view directions vary from 0° to 360° only, a slider-bar can be reasonably used to select a desired variable value. A typical slider-bar is shown in Figure A-6. A slider-bar has a title, a position indicator, and a slider button. To move the slider-bar, press the slider-bar button while holding down the left mouse button, and drag the button to the desired position. It is also possible to press on the gray area to either side of the slider-bar button. This will move the slider-bar button 1/10th of the total range of the slider-bar in the indicated direction (i.e. ±36° for the above example).

Note that with slider-bars, the desired value is not always exactly attainable. Slider-bars are limited to 100 positions. This means that with the view directions mentioned above, the smallest angular step is 3.6°.

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Slider Bar

Figure A-6 X- windows/Motif slider bar

Slider bars are useful for selecting variable values which fall within a specified range. For example, the slider bar may be used to specify the percent (0% to 100%) red that should be used if defining a new color. The range of possible answers is restricted.

G. TEXT FIELDS:

Text fields are used to enter new variable values. The format of a text field is shown in Figure A-7. The field is composed of the variable name and a recessed text entry box. To enter a new value in the entry box, select the text field with the mouse button, erase the previous entry and type in the new entry. To enter the new value press <RETURN> when done, or press *OK* or *Apply* if the text field is part of a pop-up dialog

box. There are a variety of ways to erase a previous entry. The user may position the insert cursor at the end of the current entry and *Backspace* over the old entry. The user may also quickly double-click with the left mouse button in the text field, highlighting the entire selection. The next typed key will replace the highlighted selection. The user may also start at one end of the selection, hold the left mouse button down, and drag the mouse over the rest of the selection. This will highlight the entire selection; the next typed key will replace the entire highlighted selection.

Text Field: | 12.344110 |
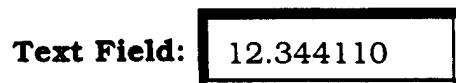
Figure A-7   X-windows/Motif text field.
A text field is used to display current variable values, and allow the user to enter new values.

H. TOGGLES:

Many program options are either *ON* or *OFF*, *TRUE* or *FALSE* or Toggle Buttons. Toggle buttons are very useful for defining variables or parameters. Two toggle buttons are shown in Figure A-8, the top one is *OFF/FALSE* and appears raised, and the bottom button is *ON/TRUE* appearing recessed. To the right of the toggle is the description. Toggle buttons are always squares. The selection is changed by pressing the toggle button.

☐ **Toggle Button - OFF/FALSE**
☐ **Toggle Button - ON/TRUE**
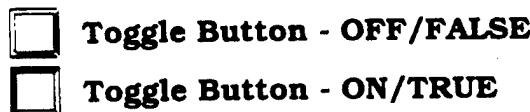
Figure A-8 X-windows/Motif Toggles.
Toggles are used to set variables to either TRUE *or* FALSE, *or* ON *or* OFF. *A raised button indicates the variable state is* FALSE *or* OFF. *A depressed button indicates the variable in* TRUE *or* ON.

I. TOGGLE MENUS:

Many variables must be set to one possible option out of several possibilities, (e.g., the line color can be red, blue, or green). These variables are defined with a toggle menu. A toggle menu can have only one active selection at a time. A sample toggle menu is shown in Figure A-9. It has a menu title, followed by a series of diamond shaped toggles. The active toggle or selection appears recessed, the rest raised. To select a menu option press the toggle next to the desired description. This activates the new selection and the previous selection will be turned off.

Toggle Menu

◇ **Option A**

◇ **Option B - Active**
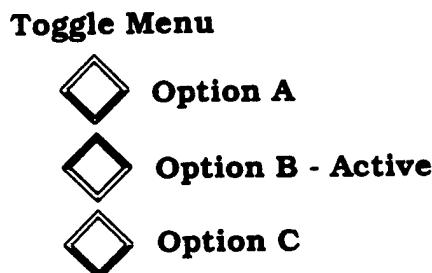
◇ **Option C**

Figure A-9 X-windows/Motif Toggle menu.

Toggle menus allow the user to select one preferred state, from among a list of options. Only one option may be chosen at a time. The recessed toggle button is the active option. Selection Dialog, *double-clicking on a filename highlights the selection and passes the filename back to the program for further processing).*

SECTION III
THE I/A-Site MAIN MENU

A. INTRODUCTION

The I/A-Site main menu is a simple user interface designed to provide easy access to all of I/A-Site's tools from one menu; however it is not the only way to access all of the tools. The experienced user will find that all of the programs in the main menu can also be started by typing the appropriate program name in an X-Window terminal. In some cases, this can be more powerful and faster than selecting choices from the pull down menus. For example, through the use of command line options and Unix shell scripts, the user can automatically process semi-variograms.

The main menu is divided into five different submenus. They are: File, Visualization, Geostatistics, Tools and Help, as shown in Figure A-10. Each of these submenus offer menu choices that provide access to programs or options in that group. As discussed in Section , to activate a menu selection, point at the desired item and hold the left mouse button down. When the item is selected a pull-down menu will appear. Continuing to hold the mouse button down, point to the desired menu choice and release the button.

In the remainder of this section, each of the five submenus in the Main Menu will be described.

Figure A-10 I/A-Site System Main Menu.

B. THE FILE MENU

The choices in the File menu are *SCO Editor, Set Directory* and *Quit.* The *SCO Editor* is a simple text editor which can be used to prepare or modify some of the data

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files used in the I/A-Site programs. Before beginning work, the project directory should be set with the *Set Project Directory* menu choice. When the directory is set, I/A-Site will place all created files in that directory and any executed programs will look for data files there. Figure A-11 shows the *Set Project Directory* dialog. The project directory is selected by pointing with the cursor to the desired directory in the *Directories* list and double clicking the left mouse button. The *Files* list will display the files in the current directory. Once the directory is selected, click the *Change* button at the bottom of the dialog to change the current working directory. The *Quit* option simply exits I/A-Site.
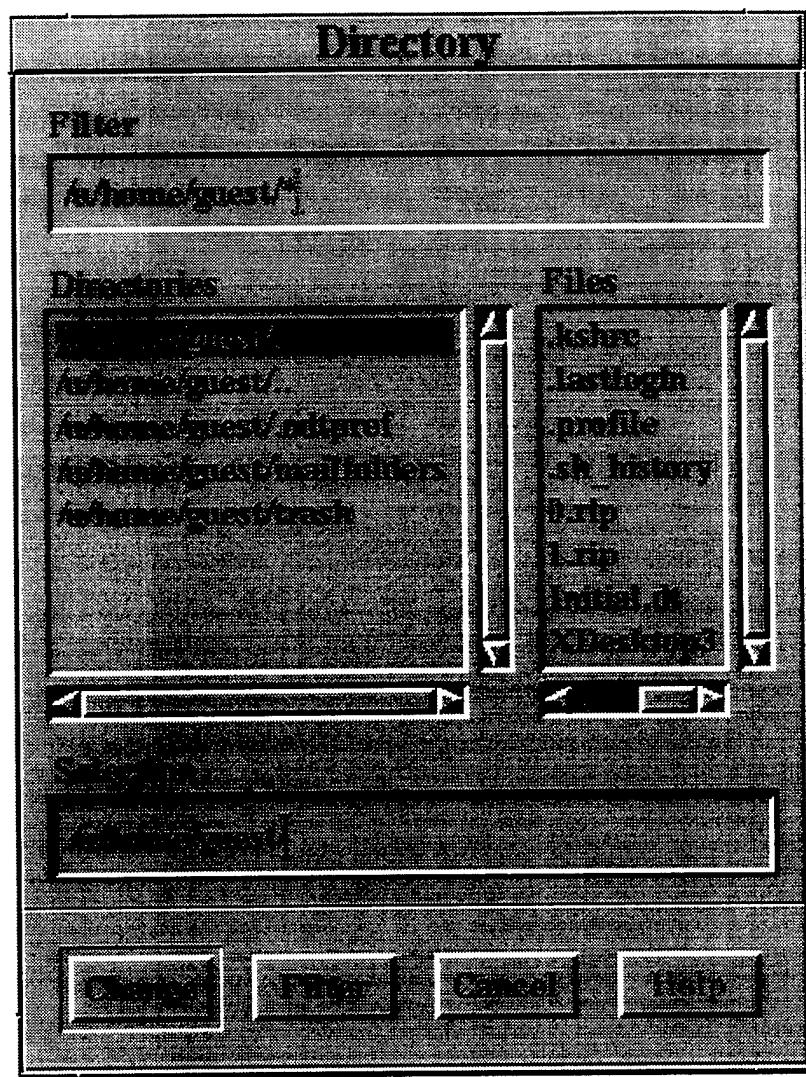
Figure A-11   Set Project Directory Dialog

C. THE VISUALIZATION MENU

The only choice in the Visualization menu is SitePlanner™. SitePlanner™ is the system database and primary visualization tools for I/A-Site. There are, however, other visualization tools available in the I/A-Site system. The UNCERT suite includes contouring, surface, 3D block, x-y plotting, and mesh viewing programs. These are all accessible through UNCERT's Visualization menu or can be started by typing the appropriate program name in a UNIX shell. The use of the UNCERT visualization tools is discussed in detail in the UNCERT User's Guide.

SitePlanner™ can be started by selecting the *SitePlanner* menu item from the Visualizations menu. If you are using the SCO Open Desktop as your working environment, there is a SitePlanner™ icon in the applications folder. Double clicking on this icon will also start SitePlanner™. Using this icon will start SitePlanner™ in the users directory instead of the project directory. Another way to start SitePlanner™ is by simply typing "siteplanner" in any UNIX shell.

Another visualization tool included with the system is ConSolve's SiteView™. This is similar to SitePlanner™ and can create 3-dimensional iso-shell surfaces. Because this program can not be used in the UNIX operating system, the user must shutdown the UNIX operating system (see SCO System Administrator's Guide), and restart the computer in DOS. SiteView™ is accessed from the Windows Program Manager.

D. GEOSTATISTICS MENU

The Geostatistics menu provides access to the main tools of the I/A-Site system. The items in this menu, shown in Figure A-12, are PLUME, UNCERT, POWDER, SCANN, and OSCAR.

PLUME is a tool based on Bayesian analysis and indicator spatial statistics. It is used to select the next sampling location based on current information about the site. Selecting PLUME from the geostatistics menu will start PLUME displaying its main menu. For more information on PLUME see Section IV.E and the PLUME documentation.

UNCERT is a collection of tools for uncertainty analysis in hydrogeologic investigations being developed at the Colorado School of Mines. Selecting UNCERT from the Geostatistics menu will start UNCERT's main menu program, positioning it directly below the I/A-Site menu. The user is referred to the UNCERT User's Guide (1) for more information on UNCERT's programs.

POWDER is a tool designed for the purpose of selecting boring locations. Selecting POWDER from the Geostatistics menu will start a program titled "powder" which is a graphical user interface (GUI) for POWDER2 written specifically for the I/A-Site system. POWDER2 and powder are discussed more in Section IV.G. and in the POWDER2 User's Guide(2).
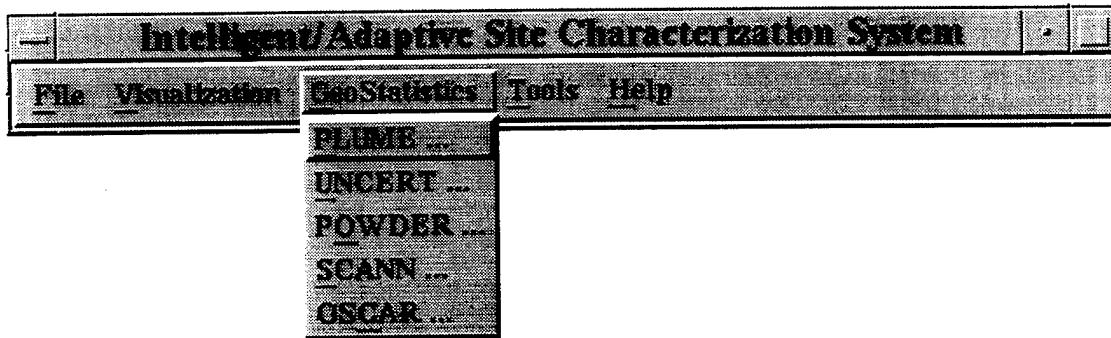
Figure A-12. Geostatistics Menu items.

SCANN is an artificial neural network (ANN) program used for interpolating field data. Selecting SCANN from the Geostatistics menu will start a program titled "scanmenu" This program is a GUI which makes running SCANN easier. SCANN and scanmenu are discussed in Section IV.H and the SCANN User's Guide (3).

OSCAR is a geostatistical tool which helps determine the economic benefit of the next sampling location before any samples are collected. Selecting this choice will start a program titled "oscarmenu" which is a GUI for the OSCAR program. The OSCAR GUI and OSCAR program are discussed in Section IV.I.

E. THE TOOLS MENU

The Tools menu has two choices: Xess™ and a Calculators submenu. The calculators submenu has three choices: UNCERT's calculator and two versions of the XCalc calculator included with UNIX X-Windows. The menu choice X:Calculator (TI30) starts *xcalc* , the program, with an interface similar to the Texas Instruments TI30, and the menu choice (HP10) starts *xcalc* with an interface similar to the Hewlett-Packard HP-10C.

Xess™ is described in detail in the Xess™ User's Guide which is included with the I/A-Site system. UNCERT's Digitizer is useful for digitizing maps if the user has a digitizing tablet connected to the computer. This program is discussed in the UNCERT User's Guide.

F. THE HELP MENU

Help provides some basic information about the I/A-Site system. This information is very limited and the user is referred to this manual and the manuals included with each software component.

SECTION IV
THE I/A-Site PROGRAMS

A. INTRODUCTION

Since one objective of this project was to use commercially available or public domain software, most of the information about the different products is contained in reports or user's guides specific to the products. The information provided in this section emphasizes how a product relates to the I/A-Site system and is not a duplication of the information provided in the user's manuals or reports. To use the tools provided in this system, the user must read and understand the documentation relating to the specific software.

B. SITEPLANNER™

SitePlanner™ is the heart of I/A-Site's data management and visualization. It is a visually accessed object-oriented database that allows the engineer to store all of the site data in an organized fashion. Object oriented means that every bit of information put into the system is an object. These objects have information associated with them. For instance, a boring may be an object that has an X and Y coordinate and a surface elevation. A sample from that boring is also an object that has as information: the source from where it was taken (the ID of the boring), a depth and chemical information. Objects can have any information the engineer wants to include. Sample objects may have additional data, such as when the sample was taken and who collected it.

SitePlanner™ can be started from the Visualization menu on I/A-Site's main menu. It can also be started from the SitePlanner™ icon if you are using the SCO Open Desktop environment, and by entering the word "siteplanner" in any of the UNIX shells. If SitePlanner™ is started from a UNIX shell, do not use this shell for anything until SitePlanner™ is exited.

Before attempting to use SitePlanner™, read the SitePlanner™ User's Guide (4) and the Reference Manual. These documents are supplied with the I/A-Site system. ConSolve also offers training courses on the use of SitePlanner™ which are very beneficial.

C. UNCERT

UNCERT is an uncertainty analysis and geostatistical software package. It adds a broad collection of tools to the I/A-Site system. UNCERT can be started from the Geostatistics menu on I/A-Site's main menu. UNCERT can also be started by entering the word "uncert" at any UNIX shell prompt. This will start UNCERT's main menu which provides access to all of the tools; however all of UNCERT's tools are even more powerful if accessed individually from a UNIX shell. Running each of the modules is discussed in great detail in the UNCERT's User's Guide.

D. PLUME

PLUME is a geostatistical tool designed to assist in the selection of sampling locations to delineate contamination events using a combination of Bayesian analysis and indicator spatial statistics. The theory, methodology and use of PLUME are discussed in the PLUME User's Manual (5). PLUME can be started from the Geostatistics menu on I/A-Site's main menu or by typing "PLUME" in any UNIX shell; however, this is not the recommended manner to start PLUME. PLUME relies on SitePlanner™ for visualization and can be linked with SitePlanner™ to access the data stored in SitePlanner's™ database. SitePlanner™ has a facility to export data from the database to what is known by SitePlanner™ as a "User Program". A "User Program" is a program such as PLUME that is written following certain specifications to accept data through a software pipe, or link, connecting two programs. In order for this software pipe to work, PLUME must be started by SitePlanner™. SitePlanner™ will start PLUME automatically when the user attempts to export data. Follow the instructions in both the PLUME User's Manual (5) and the SitePlanner™ User's Guide (4) to start User Programs from within SitePlanner™ and utilize the link between the two programs.

E. POWDER

1. Introduction

POWDER is a program developed at the University of Vermont for the purpose of guiding the location of borings in groundwater investigations dedicated to delineating the boundary of a contaminant PLUME. The version included in the I/A-Site system, titled POWDER2, is two dimensional, is valid for confined aquifer systems and assumes fully-penetrating soil borings. The program is written in FORTRAN77 and consists of four modules, although only two are supplied with the POWDER2 package. The other two are supplied with the I/A-Site system. The first module performs a variogram analysis on the hydraulic conductivity data. This module was not included with POWDER2 because the UNCERT software contains a sophisticated variogram analysis package and the user should use the UNCERT programs *vario* and *variofit* (see the UNCERT User's Guide) to perform this task. The second module is *consim2dFlow.f*. This module generates simulated velocity fields that are consistent with the observed field data using conditional simulation. The third module uses the simulated velocity fields to generate the possible contaminant distributions. This module is supplied by the user; it can be any transport model that can read the velocity field file. In the I/A-Site system, the transport model is MT3D. MT3D is a modular three-dimensional transport model developed by S. S. Papadopulos & Associates, Inc.. MT3D is used in the transport module because it is a widely used model and a graphical user interface is included with the UNCERT package. If the user wishes, they may substitute any transport model that will read the velocity output file from *consim2dFlow.f*. For more information on the use of MT3D, the user is referred to the MT3D User's Guide and the UNCERT User's Guide. The fourth module, *plumeanalysis.f*, performs an analysis of the contaminant distributions and the uncertainty data from the conditional simulations and selects the location of the next sample.

The POWDER2 manual (2) discusses the theory, program modules, running POWDER2 in character mode and the input file structure. The POWDER2 software was written to run from a UNIX shell prompt in character mode. As part of the I/A-Site project, a graphical user interface (GUI) was developed for POWDER2 to make the task of setting up input files and running simulations less tedious. The GUI is a "front end" for the original codes and simply creates the necessary files and executes the POWDER2 programs. The original programs were modified very slightly to work with the "front end"

and can still be used. The remainder of this section discusses I/A-Site's GUI for POWDER2.

2. I/A-Site's POWDER2 GUI

POWDER2 GUI is started from the I/A-Site main menu in the Geostatistics menu or by typing the word "powder" in any UNIX text shell. The main menu for the POWDER2 GUI is displayed in Figure A-13. The POWDER GUI has six choices in the main menu. They are File, Parameters, Run, Tools, Log and Help. The File menu only has two choices: *Set Directory* and *Quit*. The *Set Directory* choice allows you to change to a different working directory and *Quit* exits the POWDER GUI. The Parameters and Run options are discussed later. The Tools menu has three choices: Xess™, Editor, and a Calculators submenu. The calculators submenu has three choices: UNCERT's calculator and two versions of the XCalc calculator included with SCOUNIX X-Windows. The menu choice X:Calculator (TI30) starts the program *xcalc* with an interface similar to the Texas Instruments TI30. The menu choice (HP10) starts *xcalc* with an interface similar to the Hewlett Packard HP-10C. Xess™ is describe in detail in the Xess™ User's Guide which is included with the I/A-Site system. The Log menu allows the user to save information displayed in the text window to a file, view the file in an editor or print it. The Help menu provides on-line information about POWDER2.
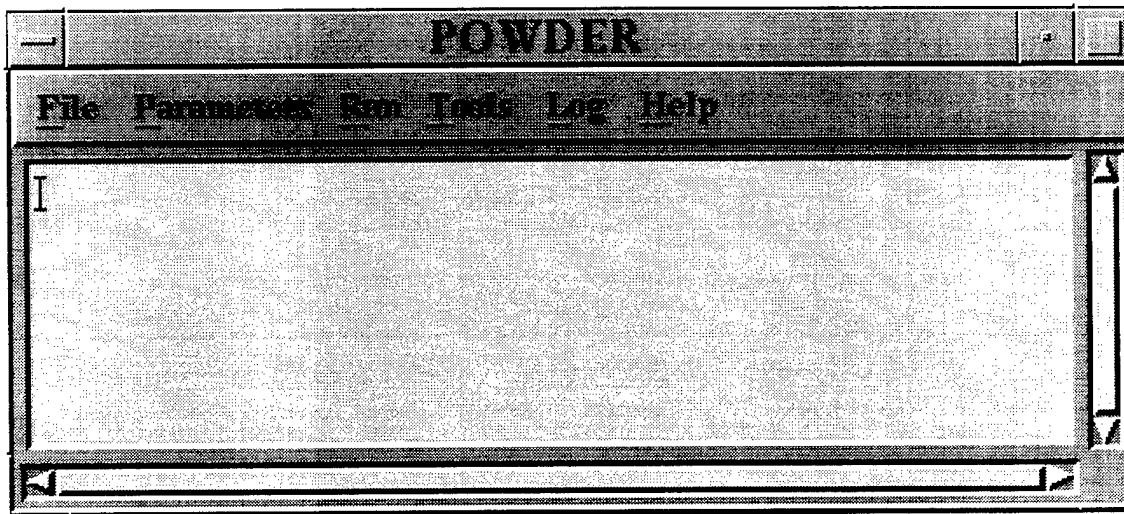
Figure A-13. I/A-Site's GUI for POWDER2.

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Creating input files and running POWDER2 is done with the choices in the Parameters menu and the Run menu. From the Parameters menu there are two choices: ConSim2dFlow Parameters and Plume Analysis Parameters. The ConSim2dFlow Parameters choice opens a dialog where the user can enter all the information required to run conditional simulaitons of hydraulic conductivity and flow. This dialog is shown in Figure A-14.
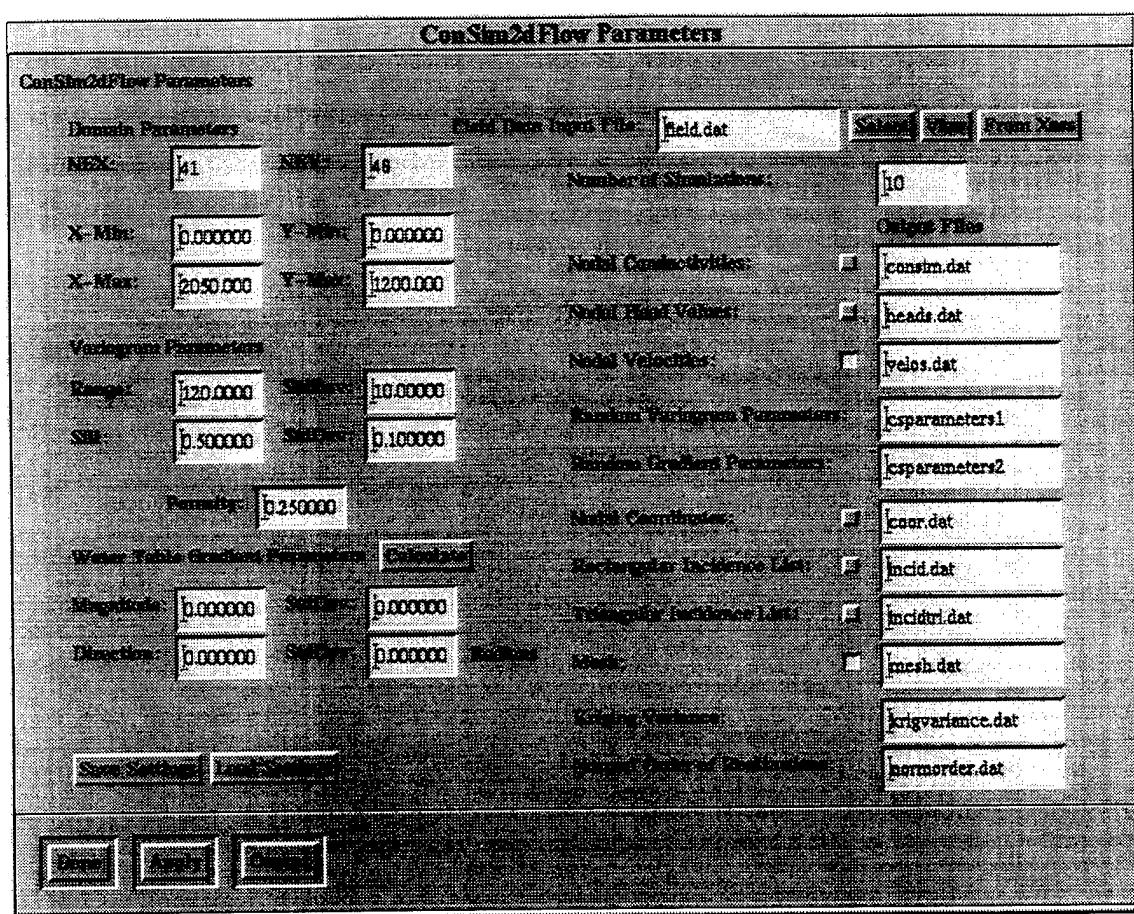
Figure A-14 ConSim2d Flow Input Parameters Dialog.

This dialog is grouped into four sections: Domain Parameters, Variogram Parameters, Water Table Gradient Parameters, and file selection. The information entered in each of these areas is used to create the *start.consim2dFlow* file discussed in Section 4.1.2 of the POWDER2 User's Guide (2). A *start.consim2dFlow* file is created when the user selects *Apply* or *Done*. Consim2dFlow is executed from the Run menu by selecting

Run Consin2dFlow. After Consim2dFlow is executed, various output files are created, as selected in the dialog's Output Files section. These files can be used as input to a contaminant transport simulator. The transport simulator is run for the set of flow simulations to create a concentration distribution for each flow simulation. When the concentration distribution is created the next step is to run Plume Analysis.

The *Plume Analysis Parameters* choice in the Parameters menu will open a dialog where the user can enters all the infromation required to run the program. This dialog is shown in Figure A-15.
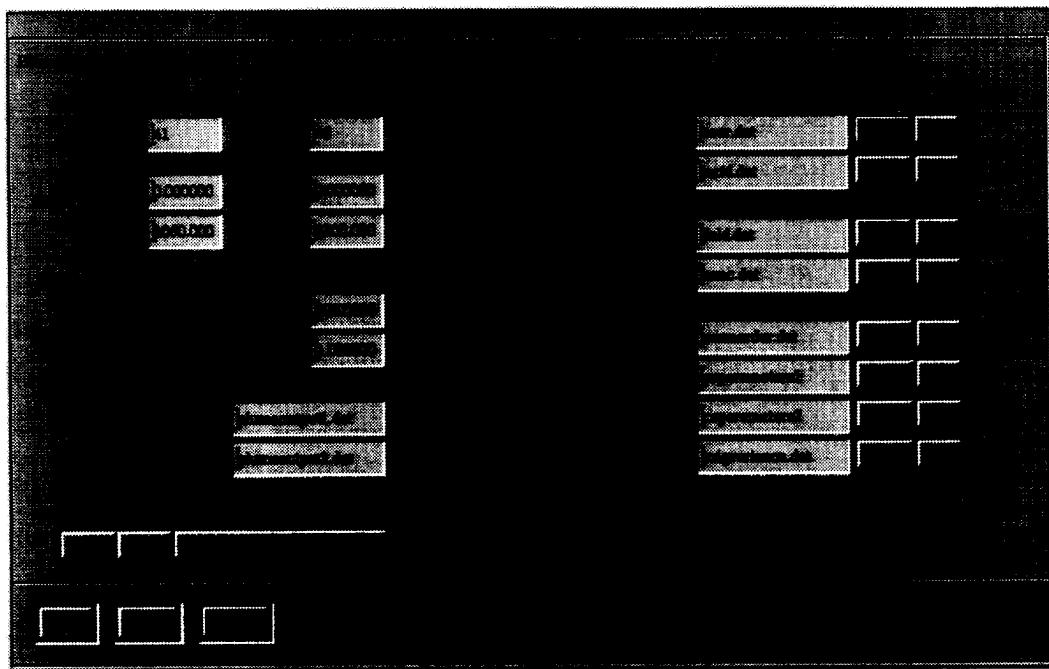
Figure A-15   Date entry dialog for POWDER2's *PlumeAnalysis* module.

This dialog is similar to the Consim2dFlow Parameters dialog and some of the required information can be read from the *start.consim2dFlow* file by selecting the *Load from Consim2dFlow* button. As with Consim2dFlow the information in this dialog is used to create the an input file. In this case, the file is*start.plumes* and is discussed in Section 4.1.3 of the POWDER2 User's Guide (2). After this file is created, PlumeAnalysis can be executed from the *Run* menu. When Plume Analysis completes, the node number and spatial coordinates of the next sample location are displayed.

F. SCANN

1. Introduction

SCANN is a program developed at the University of Vermont for solving pattern completion problems. It is usefull for creating distribution maps of field parameters such as hydraulic conductivity or contaminant concentration. The version of SCANN distributed with the I/A-Site system is capable of handeling one- two- or three-dimensional problems and is written in FORTRAN77. The SCANN User's Guide (3) contains a discussion of Artificial Neural Networks (ANN), SCANN's input/output files and running SCANN. The SCANN program was written to run in command line mode from a UNIX shell or DOS prompt. SCANN does not include a GUI or postprocessor for viewing the results. As part of the I/A-Site project, a GUI was written for SCANN along with a postprocessor to convert SCANN output files so the results can be displayed with UNCERT's graphic programs. The GUI for SCANN is discussed in the remainder of the section.

2. I/A-Site's SCANN GUI

The SCANN GUI is titled "scannmenu" and can be started by selecting SCANN from the Geostatistics menu in I/A-Site's main menu or by typing "scannmenu" at any UNIX shell prompt. The SCANN GUI has a main menu which is displayed when the program is started. As can be seen in Figure A-16 there are six choices on the main menu, File, Run, Tools, View, Log and Help.
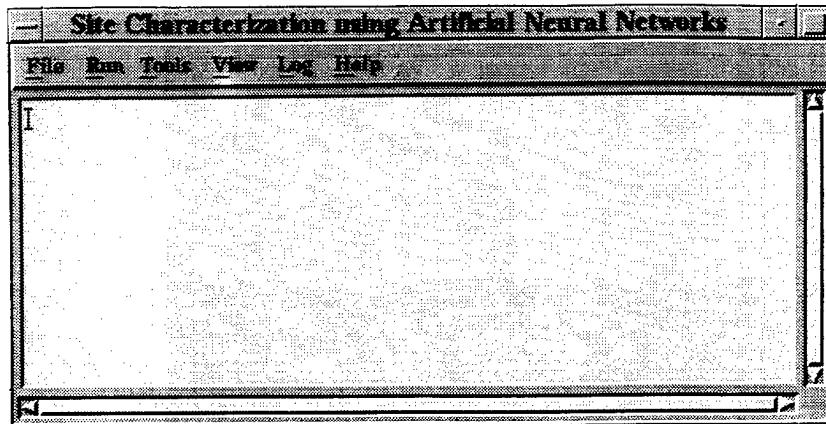
Figure A-16 The SCANN GUI Main Menu.

To run SCANN, the user selects *SCANN* from the Run menu and is presented with a simple dialog for selecting the input and output files shown in Figure A-17. The input file is created by the user in a standard text editor, like the SCO Editor, following the format specified in section 3.1 of the SCANN User's Guide. The input file has four main parts, the header, the training vector coordinates, the training vector class data, and the coordinates at which the user would like to predict values. The SCANN GUI provides a utility for generating a list of coordinates for a regular grid in the proper format for SCANN to be used in this forth part of the input file. This utility is accessed from the Tools menu and is titled *Generate Regular Grid Dialog* as shown in Figure A-18. The utility creates a file that can be added to SCANN's input file. The Xess spreadsheet applications is a very usefull tool to aid in creating other parts of the input file, for example, converting real data into categorial data. After the input file has been created and selected and an output file name is given, SCANN will run when the user selects *Done* or *Apply* from the dialog. Selecting *Done* will return the user back to the main menu while selecting *Apply* will run SCANN and leave the dialog open.
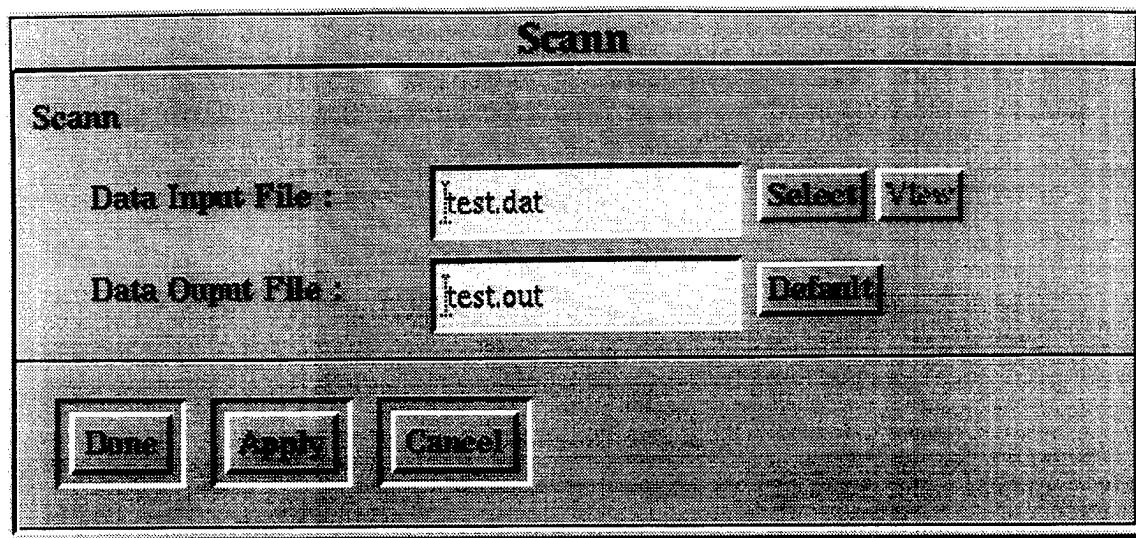
Figure A-17 Setting the Input/Output Files for SCANN.
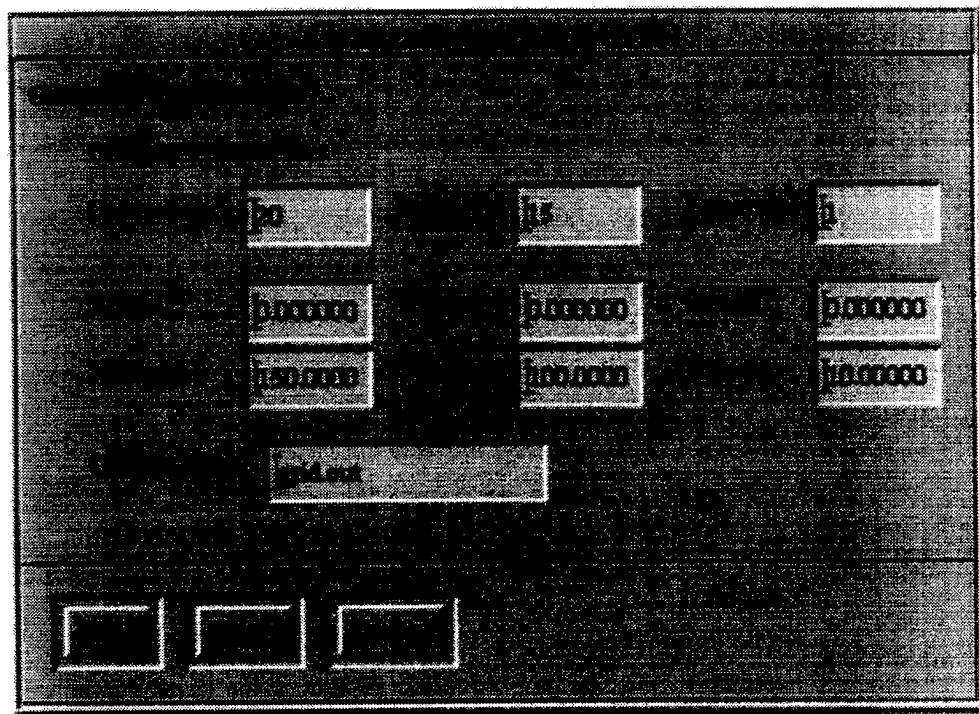
Figure A-18 Generate Regular Grid Dialog.

To view the results from a SCANN run, the output file must be post-processed. The SCANN GUI provides a post processor which is accessed by selecting *Post Processor*

from the Run menu. This utility, shown in Figure A-19 can create UNCERT or ASCII TSV (Tab Separated Value) files of the SCANN results. To create UNCERT files the user must first define the UNCERT grid definition by selecting this button on the dialog. Once the data are post-processed the user can view the results as either a contour or a surface map by selecting the appropriate choice from the View menu.
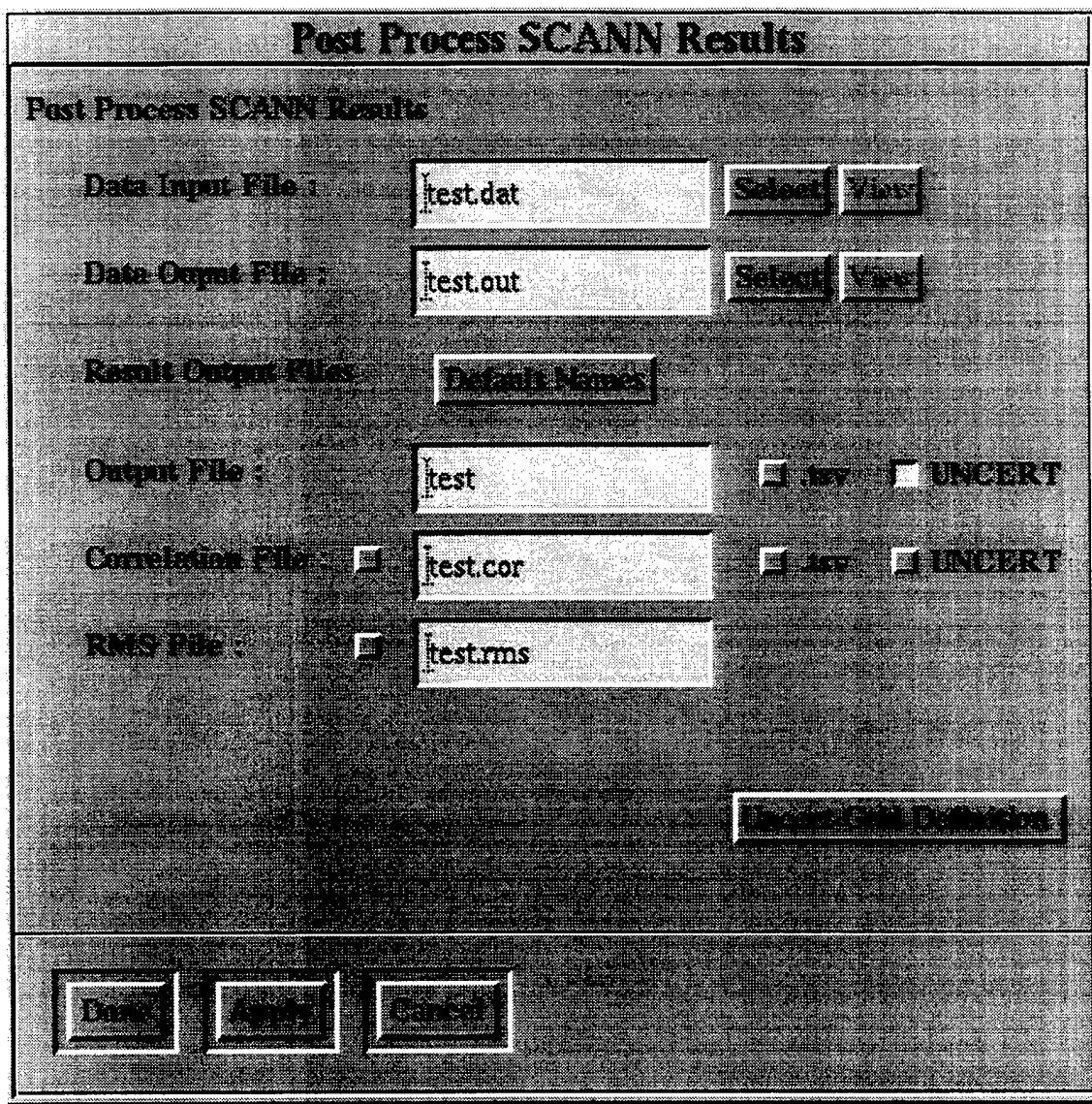
Figure A-19 Post Processor for SCANN.

G. OSCAR

OSCAR is a program developed by Applied Research Associates, Inc. for helping the engineer determine the economic benifit of the next sampling location. OSCAR is written in the C programing lanquage. A theoretical discussion of the methodology behind OSCAR is included in the OSCAR report (6).

OSCAR is accessed from I/A-Site Geostatistical menu by selecting the *OSCAR* choice. The GUI shown in Figure A-20 has a main menu with the choices File, Simulations, Tools, Log and Help. To run OSCAR the input parameters must be specified first by selecting *OSCAR Parameters* from the Simulations menu. The parameters are entered in a dialog shown in Figure A-21. After all of the required information is entered and an OSCAR input file is created the *Run OSCAR* choice is selected from the Simulations menu. The *Run OSCAR* dialog is shown in Figure A-22. Here the user specifies the name of the OSCAR input file (`oscar.inp` in this example), the location being tested and whether or not the input file is new or old. If the input file is the same as a previous simulation and the user is testing the economic benefit of a different location, selecting *Old* will cause the simulation to run faster. The results of an OSCAR simulation are stored in a text file with the same root as the oscar input file and an extension "`.out`". The results are presented as the total cost of clean up with and without the additional sample.
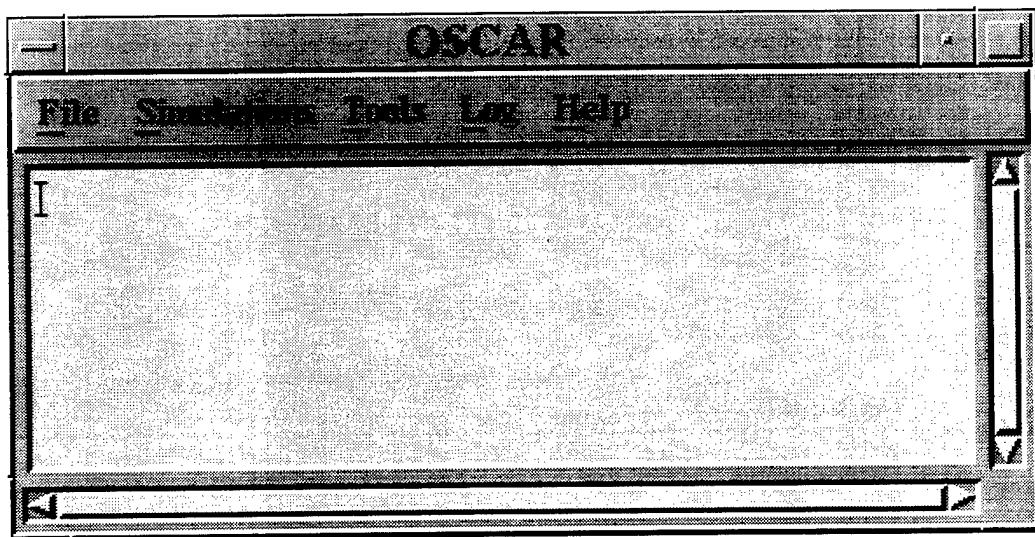

Figure A-20 OSCAR Main Menu Dialog.

Figure A-21 OSCAR Input Parameters Dialog.
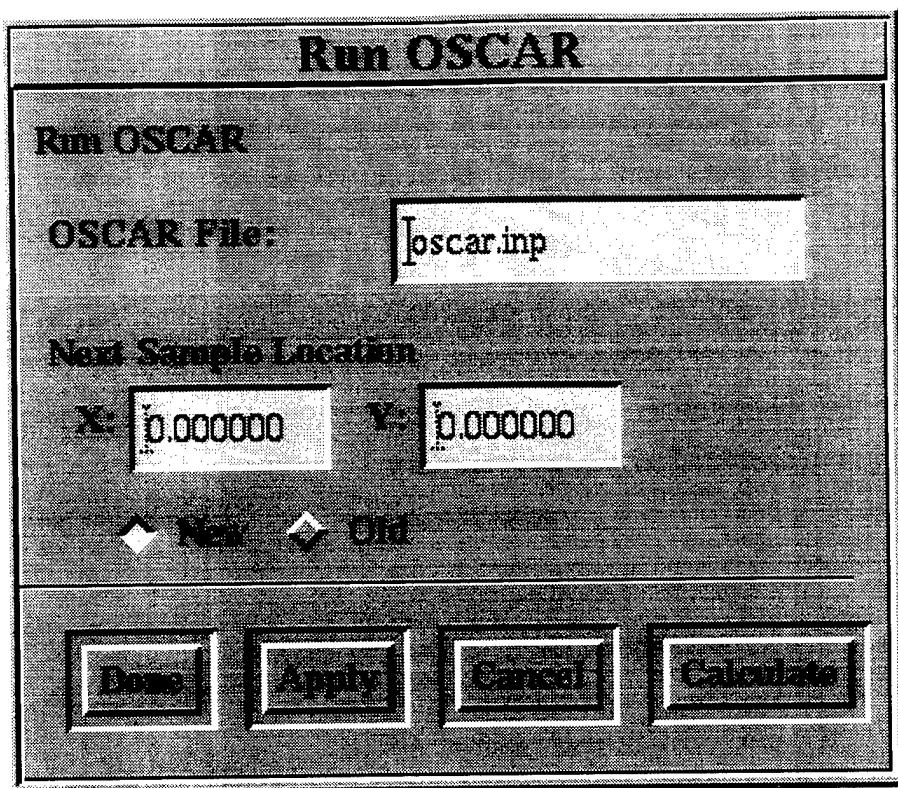
Figure A-22 OSCAR Run Simulation Dialog.

H. CONETAP

Cone Test Analysis Program (ConeTAP) is a DOS based program designed to perform a variety of functions. The major function of the program is to calculate engineering parameters from raw CPT data. These values include the direct CPT measurements and numerous engineering values which are derived from published correlations. The program will average CPT data over a specified interval and output files suitable for input into SitePlanner™. For more information on ConeTAP and specific operating instructions, consult the ConeTAP users manual.

I. SITEVIEW™

SiteView is a graphics tool developed by ConSolve, Inc. in Lexington Massachuesetts. SiteView runs on the Windows 3.1/NT operating system and therefor the user must shutdown the SCO Unix operating system and restart in DOS mode. This

procedure is discussed in the SCO System Administrators Guide. Data to be displayed with SiteView can be saved to the DOS partition on the storage device and later accessed from within Windows after restarting the computer. Use of SiteView is covered in the SiteView Users Guide.

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